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THE UNIVERSITY OF ALBERTA

Mass Transport Phenomena in Osmotic Processes; Experimental Measurements and Theoretical Considerations

by

© Michele Marcotte

A THESIS
SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE OF

Master of Science
IN
Food Engineering

DEPARTMENT OF FOOD SCIENCE

EDMONTON, ALBERTA
Fall 1988

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THE UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled **MASS TRANSPORT PHENOMENA IN OSMOTIC PROCESSES; EXPERIMENTAL MEASUREMENTS AND THEORETICAL CONSIDERATIONS** submitted by **Michele Marcotte** in partial fulfilment of the requirements for the degree of **Master of Science in Food Engineering.**

(supervisor)

R. J. Tait

Monica Palcic

DATE: July 7, 1988

DEDICATION

To Slobo,
for his incredible patience,
love and support

ABSTRACT

The osmotic behavior of potato tissue immersed in a sucrose solution has been studied. From the experimental work, the equilibrium study has shown that cell wall influences the shrinkage behavior of the tissue. A constant total final volume was found for a wide range of concentrations (10% to 40%) of sucrose solutions which seems to indicate that the cells are plasmolyzed. It was found that the extracellular space increases as soon as incipient plasmolysis is reached. Sucrose and water enter the extracellular space so that the cell structure does not collapse. There is no penetration of sucrose in the cellular volume. The experimental measurements of total cell volume, extracellular volume and cellular volume seem to indicate that there is a loss of the integrity of the cells when the tissue is in equilibrium with a highly concentrated sucrose solution (40% to 60%). A comparison between the calculated cell volumes from sorption data and the experimental volumes revealed that the calculated total cell volume matches the cellular volume obtained from experimental measurements for the whole range of sucrose solutions. Furthermore, one can predict from the sorption data the behavior of the cellular volume. Finally, it was observed that most of the loss of water from the potato tissue occurs from the vacuole of the cell.

From the kinetic study, it was found that the shrinkage pattern affects the mass transport phenomena. The variable free surface area of mass transfer (area of extracellular space) influences the depth of penetration of sugar as well as the difference in chemical potential between the potato material and the osmotic solution.

A geometrical equivalent (Toupin, 1986) was used to develop a model which describes the mass transfer of sucrose in potato material. It was found that the model proposed is able to predict the mass transport phenomena of potato tissue undergoing an osmotic treatment in a sucrose solution.

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LIST OF SYMBOLS

a	Constant of the regression equation relating the peak height versus the sucrose concentration
$\hat{a}$	Activity of constituent in solution
a_o, a_1	Constants of the regression equation relating the standard diffusion coefficient to the concentration of sucrose
A	Surface area(m^2)
$\mathcal{A}$	Constant in eq.[3.18], eq.[4.58].
A_t	Cross-sectional area of the tissue exposed(m^2)
α	Ratio of the molecular weight of water over the molecular weight of component in eq.[3.19], eq.[3.20], eq.[4.59] and eq.[4.60].
αp	Fraction of the area of the plasmalemma occupied by the plasmodesmata.
b	Constant of the regression equation relating the peak height versus the sucrose concentration.
B	Constant of the Hasley correlation eq.[3.39]
β_1	Variation of the cell wall elasticity modulus with respect to the intracellular hydrostatic pressure.
β_2	Value of the cell wall elastic modulus at incipient plasmolysis (Pa).
C_1, C_2, C_3	Constants for Ratti et al. correlation eq.[3.38].
$\bar{C}$	Concentration of sucrose ($kmol/m^3$).

C	Variable for Ratti's correlation eq.[3.36] and eq.[3.38].
c	Constant for Hasley correlation eq.[3.39]
#C	Total number of cells.
$\#C_{co}$	Number of cells in a column of cylindrical unit cells.
#co	Number of columns.
CMM1, CM, CMP1, CSM2, CSM1, CB, C0, C1 and C2	Lumped non linear terms of finite difference equations.
d	Diameter (m)
D	Standard diffusion coefficient (m^2/s).
D	Diffusion coefficient with respect to the mass average velocity (m^2/s).
$\bar{D}$	Corrected diffusivity with respect to the mass average velocity (m^2/s).
δz	Small increment of z.
$\delta\theta$	Small increment of θ.
DF	Dilution Factor.
DPM	Desintegration per minute.
ϵ	Void Fraction of the porous structure.
ξ	Elastic modulus of the cell wall (N/m^2).
FPD	Freezing Point Depression (K).
γ	Activity coefficient.
h	Space increment (m).
IS	Insoluble Solids (%).
ISL	Insoluble Solids Loss (%).
k	Time increment (s).

κ	Compliance factor.
l	Length of the cell (m).
L	Macroscopic phenological coefficient ($kmol^2/J\ m^2s$).
$\bar{L}$	Relative partial molar enthalpy.
m	mass (kg).
m	molality
M	Molecular weight (kg/kmol)
ML	Mass Loss (%).
μ	Chemical potential.
n	Number of moles (kmol)
N	Mass flux (kg/m^2s).
OP	Osmotic Pressure (Pa).
P	Hydrostatic Pressure (Pa).
$\mathcal{P}$	Permeability coefficient (m/s).
P	Partial pressure of water (Pa).
π	Pi value 3.14159.
PH	Peak Height.
q	Constant in eq.[4.11].
Q	Variable for Ratti correlation in eq.[3.36], eq.[3.37].
q_1, q_2 and q_3	Constants used in the Ratti correlation eq.[3.38].
ϕ	Non linear term for the condition at the interface between two cells.
Ψ	Water vapor activity.
φ	Matric Potential.

ϕ	Apparent diffusibility of a porous structure.
ϕL	Apparent relative molal enthalpy.
r	Correlation coefficient.
$\mathbb{R}$	Universal gas constant (J/kmol K).
Rwm	Water transmembrane flux (kg/m^2s).
Rwp	Water symplastic flux (kg/m^2s).
R	Radius (m).
ρ	Density (kg/m^3).
ρ_i	Volumetric mass of component i (kg/m^3).
SC	Sugar content (%).
SG	Sugar gain (%).
SGD	Sugar gain by difference (%).
Si	Suction potential of the cell content also equal to the osmotic pressure(Pa).
SU	Sucrose Uptake (%)
Sz	Water potential of the cell (Pa).
T	Temperature (K).
To	Reference temperature (K).
TS	Total Solids (%).
T_t	Thickness of the tissue exposed (m).
θ	Time (s).
τ	Tortuosity of the porous structure.
v	average velocity (m/s).
V	Volume (m^3).
$\bar{V}$	Partial molar volume (m^3/kmol).

$\bar{V}$	Partial massic volume (m^3/kg).
w	Weight fraction on a dry potato basis.
W	Wall Pressure (Pa).
W	Mass fraction of the wall.
WL	Water Loss (%).
ω	Weight fraction.
X	Water Content (kg water / kg dry matter).
x	mole fraction.
Y	Concentration of Sucrose (mg/ml).
z	Direction of diffusion or space variable (m).

Superscripts

*	Referring to the density of the pure component.
∞	Infinite dilution.
o	indicates a reference quantity or a quantity related to such reference.
o	Referring to a volume fixed frame of reference.
+	Referring to the cj+1-th cell.
-	Referring to the cj-1-th cell.
cal	indicates a calculated value.
eff	Effective.
exp	indicates an experimental value.
ft	Full turgor conditions.
H	Referring to the Hasley correlation.

in	indicates a quantity related to the inside of the cellular volume.
out	indicates a quantity related to the extracellular volume.
R	Referring to the Ratti correlation.

Subscripts

b	Referring to the buffer.
c	Referring to the cellular volume.
cel	Cellulose
cj	Indicates a quantity related to the cj-th cell.
cw	Cell wall.
cy	Cytoplasm.
d	Dish.
dm	Dry matter.
fs	Free space.
i	Referring to the extracellular volume.
i, j, k	Species.
in	Interface between two cells.
m	Indicates a quantity related to the transmembrane transport.
mix	mixture.
n	Referring to a quantity related to the n-th space grid.
os	Osmotic solution.
p	Indicates a quantity related to the symplastic transport.
po	Referring to a quantity related to the potato tissue.
pr	Proteins.

py	Pycnometer.
r	Residue.
s	Sucrose.
sa	Aliquot of the osmotic solution.
sos	Sucrose in the osmotic solution
st	Starch.
s	Indicates a quantity related to the surface of the cell.
v	Vacuole.
vi	Vial.
w	Water.

1. INTRODUCTION

Dehydration is the most important method for preservation of vegetables apart from freezing and canning. However the removal of water may considerably reduce the quality of these products. A reduced rehydratability as well as unfavorable changes in color, flavor and texture are the most common quality defects of the final products (Karel, 1975). The most common drying processes used are air drying, vacuum drying and freeze drying. All of these processes usually involve high operating costs as compared to other unit operations.

Several studies were initiated to improve the quality of the dried food by immersing the material in a suitable solution of compound prior to dehydration. The process of drying a plant material immersed in an osmotic solution has received increasing attention. It is regarded as a potential alternative or supplementary operation to conventional drying or freezing processes. The process called osmotic dehydration is an intermediate step prior to drying, dehydrofreezing and freeze drying (Ponting et al., 1966; Farkas and Lazar, 1969; Ponting; 1973; Hawkes and Flink, 1978).

Many authors have studied different aspects of osmotic dehydration, such as the choice of the solutes and their concentration in the osmotic solution, the temperature and time of the treatment, the opportunity to combine osmosis with other stabilizing techniques and the quality of the final products.

Some of the stated advantages of direct osmosis in comparison with other drying processes include minimized heat damage, less discoloration of fruit by enzymatic browning (Ponting et al. 1966; Contreras and

Smyrl, 1981), increased retention of volatiles (Flink and Karel, 1970) improved textural quality (Shipman et al. 1972) and low operating costs (Bolin et al., 1983).

Karel (1975) reported that, to a certain extent, the immersion of the plant material in an osmotic solution acts as a barrier to the entrance of oxygen.

Chirife et al.(1973) have noted the importance of the solids concentration on the retention of volatiles. Flink(1975) has shown that the retention of volatiles is increased by introducing an osmotic treatment prior to freezing as compared to a freeze dried product. From an organoleptic point of view, the products after immersing fruits in concentrated sucrose solutions are of higher quality than those without osmotic treatment. Particularly for fruits, the increase in the sugar/acid ratio after osmosis results in a pleasing sweet taste (Dixon et al.,1977). Taste scores reported by Hawkes and Flink(1978) verify the acceptability of apple slices concentrated by sucrose osmotic solutions.

As reported by Bolin et al.(1983), one of the more energy efficient means of removing moisture from a food piece is by osmosis, since water does not go through a phase change.

Shipman et al.(1972) have shown that the immersion of celery in a glycerol solution prior to air drying improved the textural quality of the rehydrated product as compared to the freeze dried or air dried products.

The quantity and the rate of water removal depend on several variables and processing parameters. In general, it has been shown that the weight loss in osmosed fruit is increased by increasing the solute concentration of the osmotic solution, the immersion time, the temperature and the solution/food ratio.

Numerous authors have pointed out the important role that the biological structure may play as a living material in the mass transport phenomena of osmosis. Osmotic water removal from fruits is possible because the cell membranes are semi permeable and allow for water to pass through them more readily than sugar. Stahl and Loncin(1979) indicated that cell walls and membranes can influence the rate of transport of cyclohexane in potato tissue. Giangiacomo et al.(1987) have emphasized the fact that the dynamics of sugar exchange between the syrup and fruit during osmotic dehydration is not only related to diffusion but is a complex process involving the original sugars and the enzymatic activity. They have also observed major differences in mass transport phenomena between fruits. Consequently, the task of estimating the process parameters becomes more difficult.

Very little has been done in the area of modelling the mass transport in plant material during osmosis. It is well known that when a solid material is placed in a solute containing environment, the solute will be transported through the solid by a diffusion process. Crank(1875) has made a detailed theoretical description of the diffusion process. From this, many attempts have been made to model the osmotic behavior (Hawkes and Flink, 1978; Conway et al.,1983). Particularly, Soddu and Gioia(1979) have used the second order Fickian equation with a diffusivity corrected by the void fraction and the tortuosity in order to model sugar diffusing in sugar beet tissue. They found that the prediction was unsatisfactory in the case of fresh beets. However, better agreement was observed for badly damaged beet. Conway et al.(1983) have used also the diffusion equation with an empirically corrected diffusion coefficient. Beyond transport related to diffusion, it is possible for other mechanisms to be of importance with respect to overall mass transport in case of an osmotic treatment.

An alternative approach is to recognize the actual cellular tissue structure of the foodstuff and to develop a predictive equation. A formal description of the tissue structure in the modelling of the drying of plant material was examined by Crapiste et al.(1984). Some work has been done on the modelling of the fundamentals of water relations in plant tissue but most of these models were developed to describe the behavior of the tissue between full turgor and zero turgor pressure and allow only for the water accounting (Philip, 1958abc; Molz and Hornberger, 1973; Molz and Ikenberry, 1974; Molz, 1976; Molz, 1979). The first attempt at modelling the mass transport phenomena in plant material upon osmosis was done by Toupin(1986) taking into account the cellular structure of the tissue.

The objective of the present study was to investigate the osmotic behavior of a simple system e. g., the treatment by immersion of potato tissue in a sucrose solution from an experimental point of view and a modelling point of view. The experimental work was divided into two parts: the equilibrium study and the kinetic study. The equilibrium study was performed to monitor the shrinkage of the potato tissue as well as to determine the equilibrium concentration of sucrose in the structure, whereas the kinetic study was conducted to establish the spatial distribution of water and sucrose inside the plant material. A model was developed taking into account the cellular structure of the potato tissue. Validation of the model was done by comparing the experimental sucrose concentration values of the slices to the calculated sucrose concentration value of the slices for a 1 hour osmotic treatment in a 60% sucrose solution at 40°C.

2. REVIEW OF THE GENERAL ASPECTS OF AN OSMOTIC TREATMENT

In this review, applications of the principle of osmosis for food processes will be presented with particular attention to osmotic dehydration. The osmotic water removal process will be defined. This will be followed by a discussion of some important parameters involved in the osmotic process such as the pretreatments, the temperature and the time of the treatment, the composition and the concentration of the osmotic solution, and the properties of plant materials. Finally, existing models will be outlined.

2.1 Applications of the Osmotic Process in the Food Area

The applications of the principle of osmosis to food processes for dehydration or freezing purposes have been primarly motivated by economical factors (Bolin et al., 1983) and the quality improvement of the final products (Flink, 1975). Although osmosis has been known for ages, in recent years there has been an increasing interest in the process.

The preservation of food, particularly vegetables and fruits, is mostly done by dehydration. Dehydrated products can be stored and transported at low costs. However, the removal of water may considerably reduce the quality of these products. Tough, "woody texture"; slow or incomplete rehydration; and loss of juiciness typical of fresh food are the most common quality defects of dehydrated food (Karel, 1975) as well as unfavorable changes in color and flavor. It is generally well known that the highest quality dry food products are produced by freeze drying. At the same time, this technique is one of the most expensive unit operations.

The process of osmosis has been proposed often as a first step followed by any kind of drying operation such as air drying, vacuum drying, or freeze drying. The plant material is immersed in an aqueous solution of certain compounds such as glycerol, ethanol, sugar or/and salt to partially dehydrate the food in order to reduce the load of water at the further drying step and to improve the quality of the final product. Today, this process is named osmotic dehydration.

Ponting et al.(1966) first suggested a process for a reduction in weight of 50% by osmotic dehydration after which the apples were either frozen, air dried, or vacuum dried. Sucrose or invert sugar were used. The advantages were superior quality product and little or no need for sulfur dioxide treatment which impairs the flavor of the product.

Farkas and Lazar(1969) initiated the study to determine the feasibility of the osmotic drying of apples prior to freezing; the conventional process being an air drying step followed by freezing. Apples were compared favorably with the conventional dehydrofrozen fruits but fruit costs would be 25%-50% higher.

Ponting(1973) observed that osmotic air dried products are high in quality immediately after drying but are unstable during storage whereas stored fruits obtained from an osmotic water removal step followed by vaccuum drying are very stable even upon storage.

Flink(1975) pointed out that the freeze dried product flavor quality depends primarly on the initial solids content and the rate of freezing. Earlier, Chirife et al.(1973) established that for low solids concentration (below 10%-20%), if the solids concentration is increased the retention of volatiles is greatly improved. When the initial solids concentration is greater than 25%, there is little effect of further increases on the retention of volatiles. An osmotic treatment of fruits in a 60% sucrose solution was used in order to increase the initial solids content prior to slow freeze drying. From an organoleptic point of view, a clear superior preference ranking was found for most of these fruits.

Hawkes and Flink(1978) emphasized that the organoleptic quality of freeze dried fruit products can be improved by increasing the solids content of the food material to levels of 25% to 35%. This also results in a reduction of the water load to the freeze drier. They also investigated the possibility of binary mixtures for the osmotic solution using the following compounds, lactose, maltodextrin, sucrose and salt mixtures.

Flink(1980) showed that osmotic concentration can be used as a step prior to freeze drying to yield food products of improved stability not only for fruits but also for vegetables. Less freeze drying time was required. Binary mixtures of salt/sugar were used.

An osmotic step also has been proposed prior to freezing. Le Maguer and Biswal(1984) suggested a dehydrocooling process. This would simultaneously cool and remove water by osmosis from vegetables before they are frozen by traditional freezing methods. Since freezing of food materials is an energy intensive process, a partial removal of water prior to this operation reduces energy consumption significantly.

Freezing methodology of fruits and vegetables using direct immersion in aqueous media has also been extensively studied (Fennema, 1973). Robertson et al.(1976) pointed out the fact that when the heat transfer fluid is an aqueous medium, such as a sodium chloride solution, the uptake of solute by the product and, subsequent solute related flavor changes and requirement for periodic replacement of the medium can be disadvantageous. They investigated the freezing of vegetables in a 23% NaCl solution. Mechanical and washing procedures were used to reduce the amount of residual freezant. Salt residuals compared favorably with the values reported for canned and remanufactured products. Preliminary cost analysis indicated competitiveness of the method to the air-blast freezing method.

Cipoletti et al.(1977) compared air blast frozen vegetables and aqueous freezant (AF) (15% NaCl, 15% ethanol) frozen vegetables. In organoleptic ratings the AF frozen vegetables were statistically indistiguishable from air-blast frozen vegetables.

Elias(1978) reported that direct immersion of vegetables in an aqueous freezant of 15% NaCl and 15% ethanol requires 25% less energy than the conventional air blasting technique. Furthermore, he found that freezing was accomplished in just 2 minutes instead of the 25 minutes exposure required by blast freezers.

Karel(1975) reported that intermediate moisture foods (I.M.F.) have received attention since the development of new products based on the following technological principles: lowering the water activity by adding a solute, such as glycerol, sucrose, glucose, or salt and retarding microbial growth by adding antimicrobial agents (primarly antimycotic) such as propylene glycol and/or sorbic acid. These I.M.F. are produced with an osmotic treatment. The initial impact of this technology was found in the area of pet foods. More recently, the development of I.M.F. for human consumption has been encouraged by the American military and the NASA.

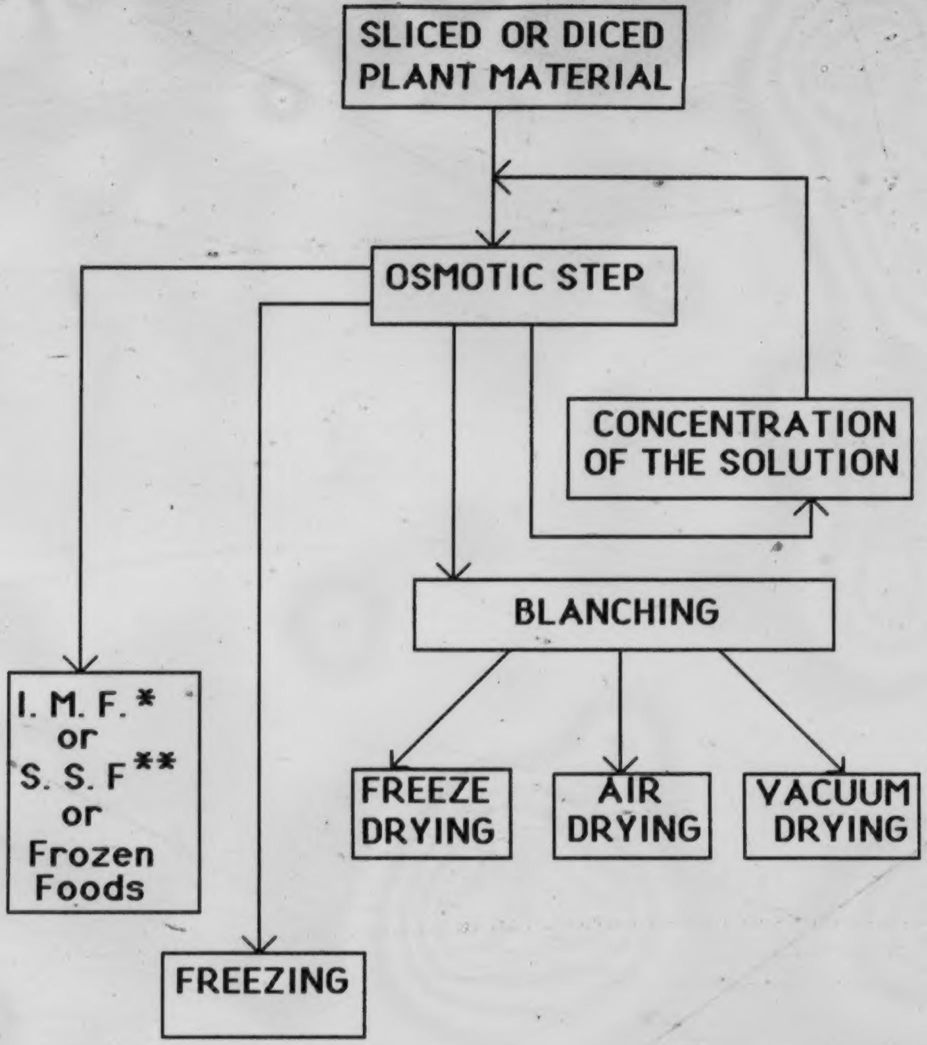
In recent years, fresh fruits and vegetables are increasing in popularity for consumption as compared to canned and frozen fruits (Shewfelt, 1987). A growing trend is emerging, however, as many of the large food processing companies have decided to market living, respiring plant tissue. In order to satisfy the growing market demand for commodities in a "fresh-like" state, minimal processings, such as low level irradiation, packaging, etc. will be increasingly used.

Maltini and Torregiani(1986) examined the possibility of obtaining, by an osmotic treatment in a sucrose solution, a shelf stable product with no need for further treatment and less preservatives. These fruit products could be eaten as they are. The product considered shelf stable shows a water activity between 0.94-0.97 and a water content in the range of 65% to 75% whereas by definition I.M.F. are foods with a water activity between 0.65-0.90 with a water content in the range of 20% to 50%. Initial contamination is of primary importance in such process but good quality shelf stable products have been obtained.

As we can see, the use of an osmotic treatment as a unit operation has already been applied widely in the food area. Fig. 2.1 summarizes a flowsheet of methods using an osmotic step for food processes.

2.2 Definition of the Osmotic Water Removal Process

According to Karel(1975) the process of dehydration of the plant material immersed in an aqueous solution is characterized by at least two major and simultaneous counter-current flows. Fig. 2.2 shows that water comes out from the biological structure to the osmoticum and solutes migrate from the osmotic solution to the tissue. There is also


SLICED OR DICED PLANT MATERIAL
OSMOTIC STEP
CONCENTRATION OF THE SOLUTION
BLANCHING
I. M. F.* or S. S. F** or Frozen Foods
FREEZE DRYING
AIR DRYING
VACUUM DRYING
FREEZING

* Intermediate Moisture Foods
** Shelf Stable Foods

Fig. 2.1 Flowsheet of Methods using an Osmotic Step for Food Processes.

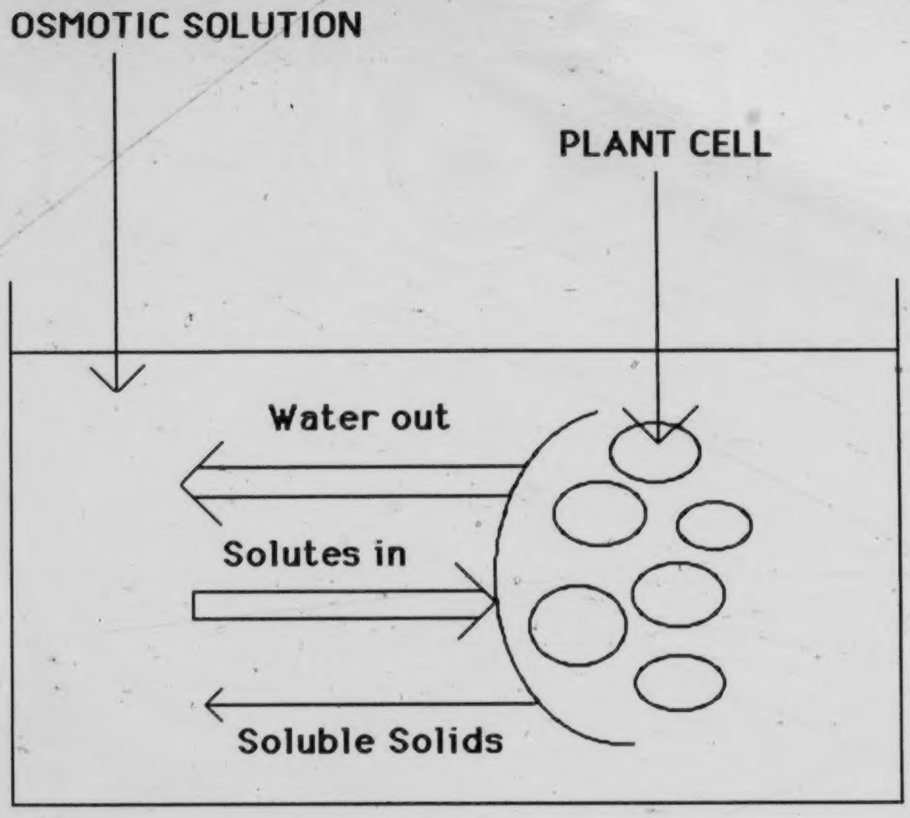

OSMOTIC SOLUTION
PLANT CELL
Water out
Solutes in
Soluble Solids

Fig. 2.2 Fluxes Involved in an Osmotic Treatment

a less important migration of soluble solutes such as organic acids, minerals and vitamins from the tissue to the osmoticum .

2.3 Important Parameters in the Osmotic Process

The characteristics of the product are controlled mostly by the history of the raw material, the temperature and the time duration of the osmotic treatment, the composition and the concentration of the osmotic solution, and finally the properties of the plant material.

2.3.1 Pretreatments

It was observed by Ponting(1973) that any treatment such as blanching or freezing prior to the osmotic water removal treatment is detrimental to the process. Osmotic dehydration is possible because of the selective permeability of the cell membranes. At this stage, killing or disrupting the cells results in poor osmosis allowing a greater uptake of sugar for a lower loss of water.

Some chemical pretreatments have been developed in order to improve the osmotic dehydration. Since drying by osmosis results in the passage of the solute into the dehydrated items which can be objectionable in some products, the concept of a membrane cast such as calcium pectate around the food to be dehydrated was developed by Camirand et al.(1968). For fruits, this coating technique was no more efficient than normal osmotic dehydration. With other foodstuffs such as fish and meat this technique proved to be very effective.

2.3.2 Temperature of the Osmotic Treatment

Ponting et al.(1966) and Lenart and Flink(1984b) found that the rate of osmosis is markedly affected by temperature. Although the rate increases with temperature, there is a limit, perhaps 60°C, above which the cell membranes are destroyed. Consequently, poor results are obtained in further osmotic water removal.

2.3.3 Time Duration of the Osmotic Treatment

Most of the studies on osmotic dehydration have been conducted in batch systems with highly concentrated sucrose solutions. Keeping the concentration of the solution constant, an increase of the contact time results in an increased weight loss or, simply, more effective dehydration (Ponting et al., 1966; Farkas and Lazar, 1969). Although the weight loss increases as a function of the time of osmosis, the rate of weight loss decreases.

Fig. 2.3. shows, schematically, how the water content and sugar concentration change with time in fruit pieces exposed to concentrated sugar solutions. The rate of water removal, which is characterized by the tangent at each point of the curve representing the water content in fruit, is maximum at the beginning of the process and the difference between the rate of sucrose uptake and the rate of water loss is maximum at the beginning of the treatment too. It is obvious that if the process is interrupted early, a considerable amount of water can be removed without a great deal of sugar uptake (Karel, 1975). Therefore the time duration of the osmotic treatment should be kept as short as possible in order to achieve a good dehydration. According to Hawkes and Flink(1978), Giangiacomo et al.(1987) and Torreggiani et al.(1987)

Fig. 2.3 has been removed due to the unavailability of copyright permission.

Fig. 2.3 Approach to Equilibrium Water and Sugar Contents during Osmotic Drying (Karel, 1975).

the maximum mass exchange takes place within the first two hours of an osmotic treatment. This is particularly significant for the design of a continuous contactor.

2.3.4 Composition and Concentration of the Osmotic Solution

The choice of the solute and the concentration employed depend upon several factors. The 2 most important factors are the organoleptic evaluation of the final product and the cost of the solute. The solubility of the solute in water is also crucial. This determines the maximum possible concentration in the osmotic solution. The capacity of the compound to lower the water activity will also affect the driving force responsible for the mass transport. Also, it is not desirable to have a solute that can react with the final product. Several studies have been done using different aqueous media. The solutes were calcium chloride, sodium chloride, ethanol, sucrose, lactose, high fructose corn syrup(HFCS) and glycerol. The properties of the solutes as well as their sensory effects on the final product are discussed.

Calcium Chloride

Ponting et al.(1972) reported that calcium treatment of apples is the usual and historical method for increasing firmness. A calcium chloride dip was effective in preserving texture over an extended storage period, as well as having a synergistic effect with ascorbic acid or sulfur dioxide in preventing browning. However, Ponting et al. (1972) observed also that calcium chloride should be used in small quantity at concentrations below 0.5% otherwise it was found to cause bitterness. This was observed also by Cipoletti et al.(1977).

Therefore, the use of calcium chloride should be limited to its preservative effects as a secondary constituent of the osmotic solution.

Sodium Chloride

According to Hawkes and Flink(1978), 25% sodium chloride is by far the best osmotic solution. It penetrates the tissue very fast thus, it increases the total solids in a very short time prior to freeze drying. However, the ability to use sodium chloride is limited by its saltiness especially in the case of fruits. Flink(1980) reported that the limiting concentration of salt in the osmotic solution, in order to have a satisfactory product from an organoleptic point of view, should probably be around 10%.

Speck(1977) found that air dried food, with an osmotic treatment in a 10% sodium chloride solution as a prestep, reached a higher degree of reconstitution than the non-treated air dried carrots. However, the calcium concentration in the tissue decreased by up to 37% due to the exchange of calcium with sodium ion.

According to Fennema(1975) polyphenoloxidases are apparently inhibited by chloride ions but the mechanism is not clear. Immersion of the cut fruits in a dilute solution of sodium chloride (1% to 3%) is a method often used during the interval between the cutting and freezing.

Lenart and Flink(1984a) pointed out the importance of the ability of the salt to lower the water activity compared to sucrose for the same level of concentration.

Ethanol

Ethanol has been used in order to decrease the viscosity and the freezing point of the osmotic solution in the dehydrocooling process as suggested by Le Maguer and Biswal(1984) and in the freezing process using an aqueous media as proposed by Cipoletti et al.(1977).

The latter authors reported that the organoleptic evaluation of the frozen diced carrots in this solution indicated a slight medicinal aftertaste caused by the ethanol. In order to block this aftertaste, predipping in a sucrose solution followed by freezing in the aqueous freezant 15% NaCl and 15% ethanol was used satisfactorily.

Sucrose

Good results have already been obtained using osmotic dehydration in a sugar solution prior to any drying or freezing operation (Ponting et al., 1966; Ponting, 1973; Farkas and Lazar, 1969; Flink,1975).

Karel(1975) reported, that to a certain extent, the immersion of plant material in a sugar solution acts as a barrier to the entrance of oxygen. Consequently, enzymatic browning is reduced.

Dixon et al.(1974) observed that the substantial increase in the sugar/acid ratio obtained in osmotic dehydration of apples as a prestep resulted in a wide appeal for the product. However, the product rehydrates only up to 70% of its original weight (Farkas and Lazar, 1969).

According to Flink and Karel(1970), carbohydrates promote the retention of volatiles whereas the ionic solute chloride does not. Mono-and disaccharides generally are more effective in promoting the retention than the polysaccharide dextran.

Finally, sucrose, being an accepted high purity food available at relatively low cost, is one of the top ranking choices. The sweetness of sucrose is one of the limitations in applications to vegetable processing.

Lactose, High Fructose Corn Syrup (HFCS) and Glycerol

Hawkes and Flink(1978) questioned the economic feasibility of using sucrose by suggesting lactose as substitute for sucrose with food materials requiring less sweetening.

Lactose may become available in increasing quantities as cheese wheys are recovered and fractionated to recover proteins, leaving a lactose rich fraction.

The solubility limit of lactose in water (around 25%) allow for the lactose to be only a partial substitute for sucrose. Even in dry system, Hawkes and Flink(1978) found that a cake layer of lactose forms a barrier around the fruit piece preventing further transport of water from the sample.

Cipoletti et al.(1977) pointed out that compounds such as sucrose, lactose etc. are not suitable for the composition of an aqueous freezant. The solution viscosity at low temperature is excessively increased.

Bolin et al.(1983) found that the rate of penetration into the fruit pieces was faster with high fructose corn syrup than sucrose. They also observed from the taste panel evaluation that sucrose solution was preferred as an osmotic medium over HFCS.

Shipman et al.(1972) have shown that the immersion of celery in a glycerol solution prior to air drying improved the textural quality of the rehydrated product as compared to the freeze dried or air dried products.

As a general rule, for the same contact time the increase of the solution concentration results in a more effective osmotic dehydration (Ponting et al., 1966; Farkas and Lazar, 1969; Hawkes and Flink, 1978).

Binary mixtures of salt and sucrose were found to be more effective than sucrose alone by Islam and Flink(1982), Flink(1980) and Lenart and Flink(1984b). They combine the properties of both solutes: capability of lowering the water activity for the salt and high water removal effect of the sucrose. The penetration of salt in the tissue, which can be organoleptically unfavorable, is limited by the sucrose. The salt hinders the shrinkage at the surface layer occurring mostly with sucrose solution immersion.

The numerous possibilities of combinations of solutes in the osmotic solution allow for its optimization in terms of maximum water removal, minimum solute gain, maximum organoleptic quality of the product, and minimum solutes cost. More recently, the findings of Giangiacomo et al.(1987) emphasized the fact that the dynamics of sugar exchange between the osmotic solution and the fruits is not only related to the mass transfer but also involves the original sugars in the fruits and the enzymatic activity. Hydrolysis of sucrose is frequently observed in fruits and vegetables, especially upon storage. Giangiacomo et al.(1987) also pointed out the importance of the relative selection of the sugars for the osmotic solution and its optimization with respect to the desirable sugar blend in the products.

From a processing point of view, the use of highly concentrated sugar solutions usually brings about two major problems. The viscosity is so large that agitation is necessary in order to decrease the resistance to the mass transfer on the solution side (Hawkes and Flink, 1978) and, because of the difference in density between the osmoticum and the tissue, the product floats in the bath solution (Farkas and Lazar, 1969).

Finally, as reported by Bolin et al.(1983), for the process to be economically feasible the solution would have to be recirculated.

2.3.5 Properties of the plant Material

2.3.5.1 Variation in the Behavior of Plant Materials upon Osmosis

According to Ponting(1973), there is a wide variation in the physical nature of fruits which is reflected in osmotically dried products. For example, because of the excessive loss of juice, tomatoes and citrus fruits are poorly suited to osmotic drying whereas it is a very successful process for apples, bananas etc.

Flink(1975) found that under the same conditions of osmosis, the increase in solids concentration in the plant material varies with respect to the kind of fruits.

Numerous authors have reported textural differences of tissue immersed in either sugar or salt solutions. Sugar is known to give a firming of the tissue and salt a softening. Lenart and Flink(1984b) emphasized that these observed textural differences should be reflected in the tissue mass transport data. The same authors pointed out that the ultimate effect of cellular dehydration on transport properties will depend on tissue properties, especially the intercellular space present in the tissue and the amount of insoluble solids.

Giangiacomo et al.(1987) observed that the difference between the data obtained for cherries and peaches under the same conditions of osmosis seems to involve the intrinsic properties of these two fruits such as the structure and the compactness of the tissue.

Stahl and Loncin(1979) investigated the diffusion of cyclohexane in potato tissue. They indicated that cell walls and membranes can influence the diffusion behavior.

Beyond the mass transport properties of the tissue, it is possible for other mechanisms to be of importance. As suggested by Lenart and Flink(1984b), the shrinkage observed in case of immersion in a sucrose solution could result in a tissue structure having reduced transport properties. More generally, any structural changes occuring during osmotic dehydration may also influence the transport properties of the tissue.

The mass transport phenomenon occuring in plant tissue upon osmosis involves complex mechanisms most of them controlled by the plant cells. In order to understand and explain this complex phenomenon, the fundamental aspects of the water relations of plant cells as established by plant physiologists now will be discussed.

2.3.5.2 Description of a Single Plant Cell

It is well known that a relative coherence exists in the plant tissue. Parenchymatous cells are the most common cell type and may form up to 80% of the total cell complement of plant storage tissue. They are the dominant type in most roots, shoots, leaves, and fruits (Hall et al., 1982).

One of the assumptions often made to simplify discussions of plant-water relations is to consider that a typical plant cell consists of a vacuole, a cell wall, and a layer of cytoplasm between the vacuole and the cell wall. The membrane which separates the vacuole from the cytoplasm (i. e., the tonoplast) and the plasma membrane which surrounds the cytoplasm controls the passage of substances from one compartment to another (Noggle and Fritz, 1976). The vacuole, the cytoplasm, and the tonoplast, and the plasmalemma constitute the protoplast. Fig. 2.4 shows the simplified representation of the plant cell.

It is generally well known that the most important organ controlling the osmosis phenomenon is the plasma membrane (Nobel, 1983). Osmosis occurs so long as solute is restricted compared to water movement. A semi permeable membrane is defined as a membrane in which the solvent molecules would penetrate readily while solute particles would not penetrate at all. The permeability is the parameter which represents the reciprocal of the resistance to mass transport across the membrane.

The turgidity of a living plant cell has a considerable significance to its physiological well-being. The elastic nature of the cell wall is important in turgor maintenance. If the cell walls were inelastic under usual changes in environmental conditions either the protoplast would separate from the wall, or if this did not occur the wall would be pulled inward with the shrinking protoplast and would buckle or rupture (Dale and Sutcliffe, 1959). Under natural growing conditions, a cell is usually at a state between zero turgor (incipient

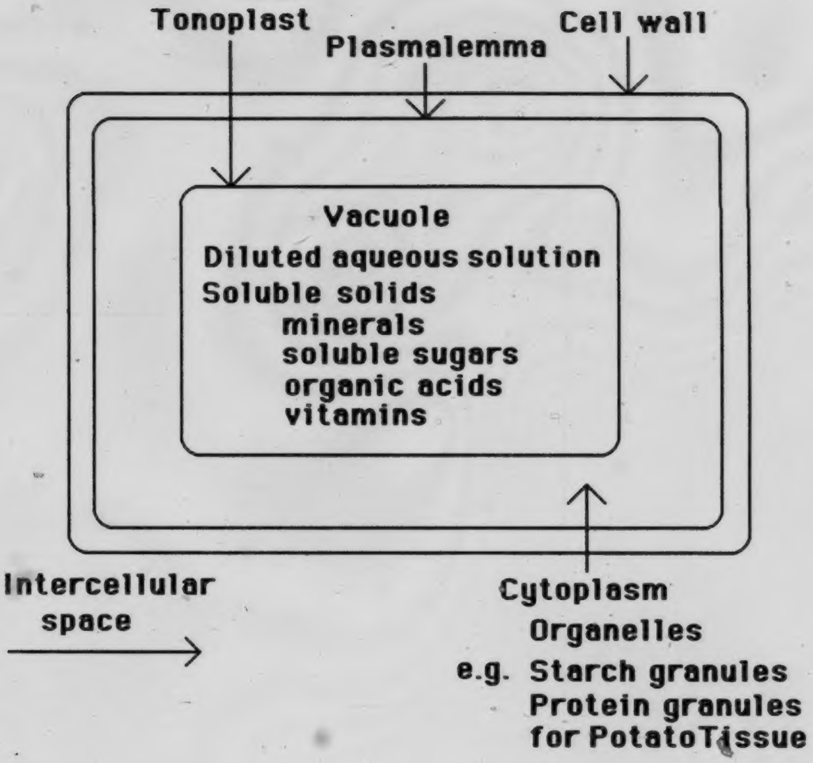

Tonoplast
Plasmalemma
Cell wall
Vacuole
Diluted aqueous solution
Soluble solids
minerals
soluble sugars
organic acids
vitamins
Intercellular space
Cytoplasm
Organelles
e.g. Starch granules
Protein granules
for Potato Tissue

Fig. 2.4 Parenchymatus Cell of Plant Material.

plasmolysis) and full turgor. Incipient plasmolysis represents the state at which the chemical potential of the cell and the outside environment are equal. It is also well known that changes in water content of plant cells occur frequently under normal changes in environmental conditions. Accompanying these changes in water content will be changes in cell volume. Cell volumes are reported to change by as much as 20%-30% (Noggle and Fritz, 1976).

2.3.5.3 Behavior of a Single Cell upon Osmosis

The description of single plant cell behavior upon immersion in an osmotic medium will now be described. Plasmolysis is a phenomenon occurring only in plant cells. It is defined as the separation of the protoplast of the plant cell from the cell wall due to the efflux of water from the cell.

An isotonic solution is defined as a solution with a chemical potential equal to the chemical potential of the cell. An hypertonic solution is defined as a solution whose chemical potential is higher than the chemical potential of the cell. When a single cell is immersed in an hypertonic solution there will be a net movement of water out of the cells and into the osmotic solution. This phenomenon is referred to as osmosis. Usually sugars such as glucose or sucrose or salts such as potassium nitrate are used to prepare plasmolyzing solutions.

Noggle and Fritz(1976) reported that a close observation under a microscope of a single cell will reveal that the cell loses its turgor in a short time; the vacuole shrinks; the volume of the protoplast decreases; and the protoplast separates away from the wall. The space between the protoplast and the cell wall becomes filled with the plasmolyzing solution. The extent of which the cell will plasmolyze is function of the concentration of the osmotic solution as it is shown on fig. 2.5. If the plasmolyzed cell remains in a certain plasmolyzing solution, it may recover from plasmolysis. The recovery will depend on the ability of the dissolved solute in the external plasmolyzing solution to penetrate through the protoplasmic layer and into the vacuole (Kedem and Katchalsky, 1958). The more rapidly the solute permeates into the vacuole, the more rapidly will deplasmolysis take place (e. g., plasmolysis with an ethanol solution).

2.3.5.4 **Transport of Water and Solute in Plant Cell**

Fig. 2.6 shows the pathway that a compound may take into a single cell from an osmosis point of view. During the passage of a substance from the outside of the plant material to its interior or vice-versa, several stages are observed. Generally the passage of solute and solvent from the external into the intercellular space and cell wall or vice-versa is readily accomplished by diffusion. Even though the plant cell wall consists of two main components, cellulose and non cellulosic polysaccharides, water forms a large portion of the cell wall. Generally, water and dissolved nutrient molecules and ions, as well as dissolved metabolites of the size of glucose, sucrose, amino acids, etc. readily diffuse across the cell wall. Only when the compound reaches the exterior surface of the protoplast of a plant cell does it encounter an effective barrier. Thus, the plasmalemma has the ability to discriminate among different chemical species and to separate the interior of the plant cell from the outside environment. Once inside

Fig. 2.5 has been removed due to the unavailability of copyright permission.

Fig. 2.5 Plasmolysis of a Plant Cell: h, cell wall; p, protoplasmic layer; k, nucleus; c, chloroplast; s, vacuolar sap; e, potassium nitrate solution (A) Section of parenchymatus cell of the immature florescence of *Cephalia leucatha* (B) Same cell in a 4% solution of potassium nitrate (C) Same in a 6% solution of potassium nitrate (D) Same cell in a 10% solution of potassium nitrate.
After de Vries (1877)
Noggle and Fritz(1976)

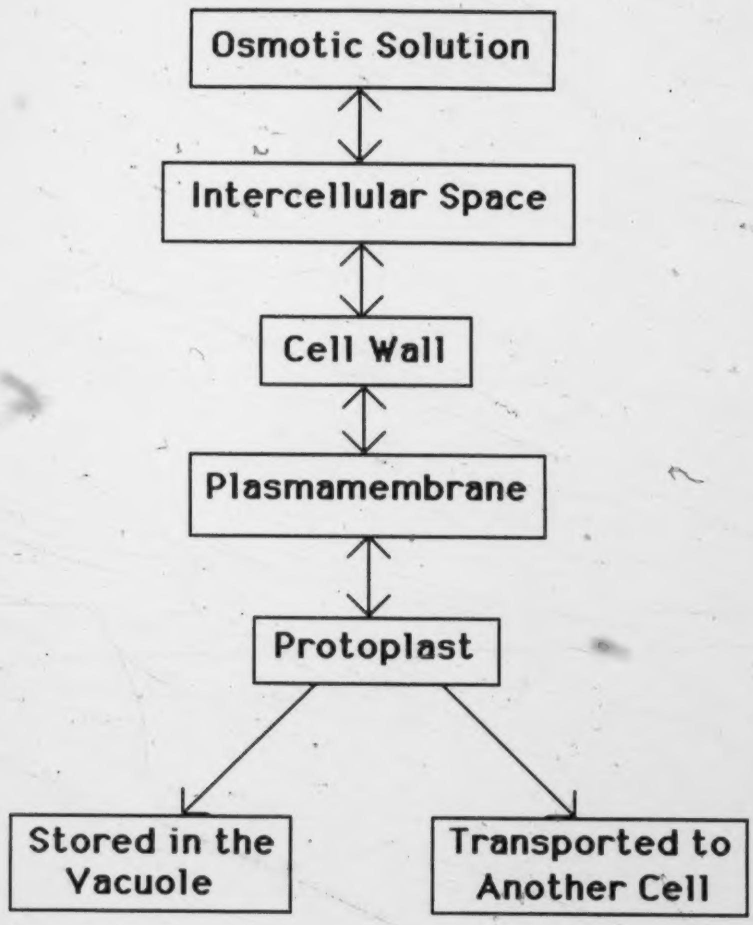

Osmotic Solution
Intercellular Space
Cell Wall
Plasmamembrane
Protoplast
Stored in the Vacuole
Transported to Another Cell

Fig. 2.6 Pathways for a Compound into a Single Cell.

the protoplast the species can be stored in the cytoplasm or in the vacuole or, it can be transported to another cell etc.

2.3.5.5 Behavior of the Whole Tissue upon Osmosis

Nowadays, although the water relations in a single plant cell is adequately described and well understood, the events are complicated when osmosis is applied to the whole plant tissue structure.

As indicated in fig. 2.7 three accepted pathways that a solute or solvent may follow while traversing a plant tissue have been identified as being responsible for the behavior of the plant material upon osmosis.

The apoplast which is exterior to the cell membrane and is visualize as a diffusion of molecules in the cell wall and the intercellular spaces between cells.

The discovery of the plasmodesmata led to another pathway. The symplast is interior to the plasmalemma and is characterized by a movement of molecules from one cell to another through small channels.

Finally, the transmembrane transport is an exchange between the protoplast and the free space which comprises the intercellular space and the cell wall.

It is obvious that the rate of swelling or shrinking of a plant tissue immersed in an osmotic solution will depend on both extracellular solute diffusion and cell membrane permeation if we consider that there is no particular relation between cells. The behavior of the whole tissue is the same as the behavior of a single cell as it is shown in fig. 2.8a. However, fig. 2.8b shows that an alternative picture is also possible when considering the importance of the relation between cells.

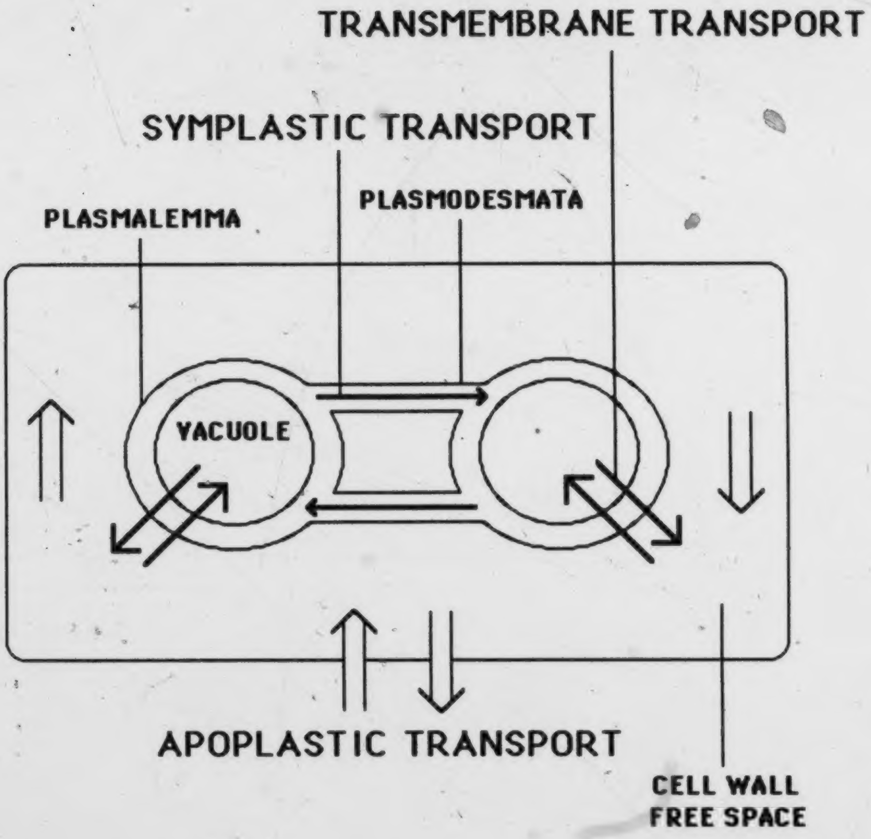

TRANSMEMBRANE TRANSPORT
SYMPLASTIC TRANSPORT
PLASMALEMMA
PLASMODESMATA
VACUOLE
APOPLASTIC TRANSPORT
CELL WALL
FREE SPACE

Fig. 2.7 Mechanisms of Mass Transfer inside the Biological Structure.

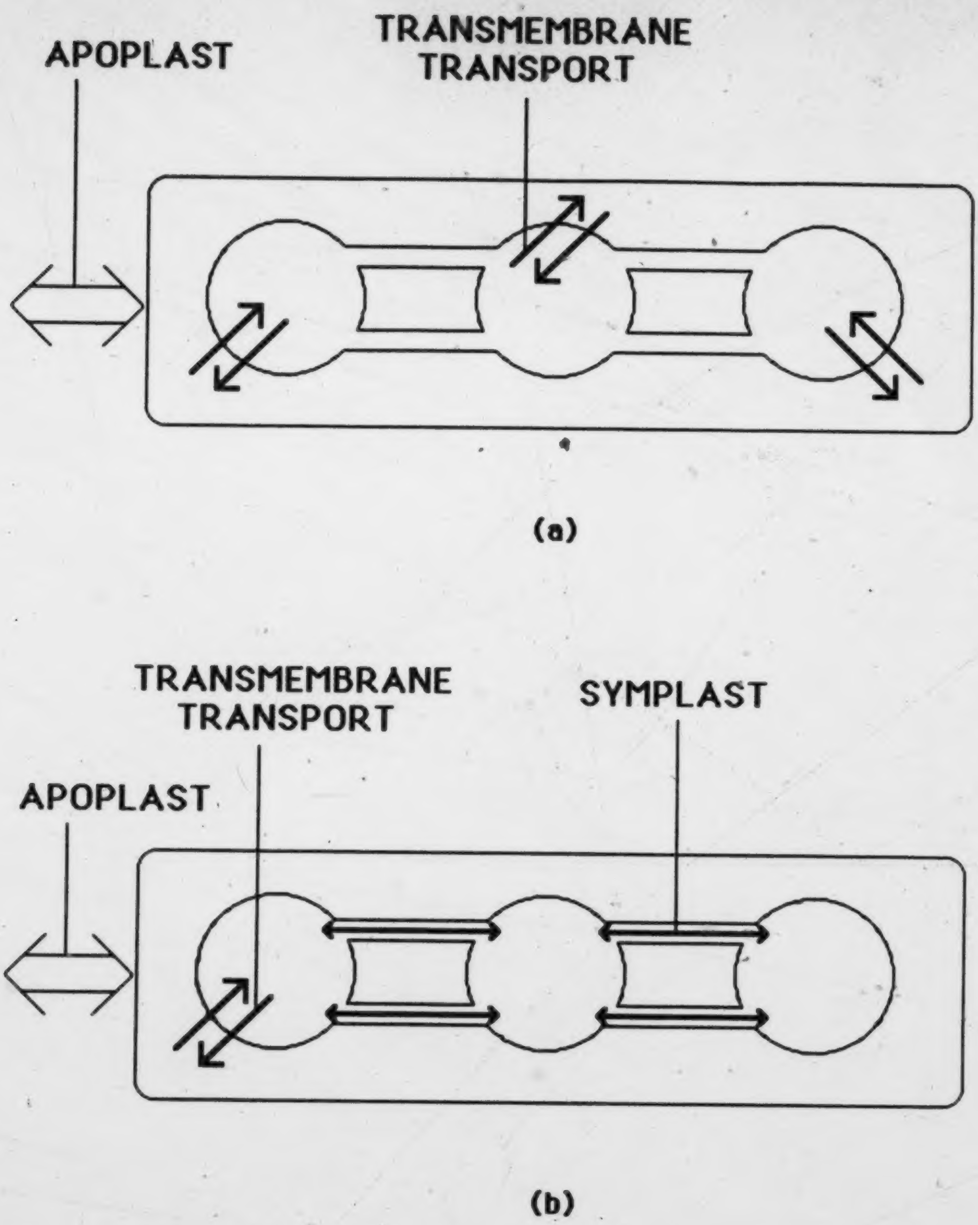

APOPLAST
TRANSMEMBRANE TRANSPORT
(a)
TRANSMEMBRANE TRANSPORT
SYMPLAST
APOPLAST
(b)

Fig. 2.8 Different Pictures for the Behavior of the Plant Material upon Osmosis.

A change in the concentration of the osmoticum is sensed by the surface of the cells and the preferential pathway for the solvent can take place entirely from cell to cell through the plasmodesmata and not through the extracellular space. Whether or not the apoplast or the symplast pathway for water is the more important in plant tissue will indicate which of the two pictures are correct. It might vary for different plant tissues.

2.4 Existing Models

When a solid material is placed in a solute containing environment, the solute will be transported through diffusion. The diffusive transfer of solutes from a solid to a surrounding solvent or vice-versa is used widely in the food industry (i. e., desalting of pickles, extraction of oil and sugar etc.).

In such processes, the molecular diffusion in the solid, which is slow, controls. Since biological tissues are essentially porous or cellular solids in which a gas and/or a liquid are immobilized in a solid matrix, the rate of mass transfer can be approximately predicted by appropriate solutions of the simplified unsteady state second Fickian equation provided that the apparent or effective diffusivity is known. The transfer is assumed to be unidirectional and the effects of the other components on the diffusion of the solute are negligible.

$$\frac{\partial \bar{C}_i}{\partial \theta} = \frac{\partial}{\partial z}\left[D_i \frac{\partial \bar{C}_i}{\partial z} \right] \qquad [2.1]$$

Crank(1975) has made a detailed theoretical analysis of the diffusion process. Analytical solutions of eq.[2.1] are available for idealized geometries (i. e., spheres, infinite cylinders, infinite slabs, and semi infinite media). For these analytical solutions of the unsteady state Fickian diffusion model to apply, it is necessary either to keep the external solution concentration constant or to have a fixed volume of solution. A constant diffusion coefficient diffusion also is assumed. The resistance at the surface of the solid is assumed to be negligible compared to the internal diffusion resistance in the solid.

If diffusion takes place in porous media the effective diffusivity is lower than the diffusion coefficient in the absence of a porous medium. In which case, we can relate the diffusivity of that species in solution to the apparent diffusivity in a porous solid by a correction factor that contains the void fraction and the tortuosity.

Soddu and Gioia(1979) tried to model the process of sugar diffusing from a beet immersed in water using a solution of the unsteady state second order Fickian equation with an effective diffusion coefficient corrected by the void fraction and the tortuosity. They found that the comparison was quite unsatisfactory, especially for the experimental data regarding fresh sugar beets. However better agreement was observed for badly damaged beets. It is obvious that when cells are viable they play a role in the overall mass transfer.

More recently, Conway et al.(1983) considered, for the purpose of modelling, that only a simple diffusion of water was occurring upon osmotic dehydration of apples in a sucrose solution. The solution given by Crank(1975) of the second order Fickian equation was used to calculate the theoretical moisture ratio and to compare with the experimentally determined ones. It was found empirically that the logarithm of the diffusivity decreased linearly with the sucrose concentration of the solution and the reciprocal of the temperature. There was also an interaction between the temperature term and the sucrose concentration of the solution.

Hawkes and Flink(1978) tried to quantify the so-called mass transfer coefficient by plotting the normalized solids content of the apple slices (percent total solids change based on the initial total solids) versus the square root of time and calculating the slope at each point of the curve in order to compare different systems (i. e., different osmotic solutions). This procedure is a standard method of estimating diffusion coefficients assuming an unsteady state Fickian diffusion in a semi infinite medium.

The conditions assumed in order to use the solution for the unsteady state Fickian equation do not necessarily simulate an osmotic process as in osmosis, there is usually more than one important flux. Also shrinkage occurs.

Lerici et al.(1985) pointed out that to characterize an osmotic treatment it is important to take into account not only the weight reduction and the water loss but also the solids gain.

Another approach was used by Guenneugues(1986) in order to model the overall mass transfer in multicomponent system occurring in plant tissue upon osmosis. In this work, mass transfer was approached from the standpoint of irreversible thermodynamics taking into account the fluxes of the different components of the system and the interactions between the different flows.

Lenart and Flink(1984b) found that the shrinkage is an important factor to be taken into account for the mass transport data calculations. Its spatial distribution inside the tissue was evaluated based on the distribution of moisture content for the slices as used by Suzuki et al.(1976) in drying. For osmosis with sucrose solution and salt solution, if the shrinkage is included in the calculations, the sugar gain levels fall and the water loss levels rise significantly.

The recent trend of including a formal description of the tissue structure in the modelling of the drying of plant material was recently examined by Crapiste et al.(1984) in their studies of air dehydration of foodstuff.

Complex mechanisms of transports such as diffusion outside the protoplast, transmembrane transfers, and interconnections between cells are known to be present and should be taken into account.

Furthermore, a lot of work has been done on the modelling of the water relations in plant tissue. Most of the models on the fundamentals of water relations in plant tissues have been developed in order to describe the behavior of the tissue between full turgor and zero turgor since it is occurring under natural growing conditions and allow only for the water accounting.

Philip(1958a,b,c) considered the water exchange between a linear aggregation of cells through their membranes. He pointed out that the assumption that diffusion and osmotic phenomena in whole pieces of tissue are analoguous to that in a single cell is not justified. The development was made for non permeating solutes.

Using the irreversible thermodynamic approach (Kedem and Katchalsky, 1958; Dainty, 1963), Molz and Hornberger(1973) extended the model developped by Philip(1958a,b,c) to include the effects of a diffusible solute.

Molz and Ikenberry(1974) developed a theory which allows for a water flux in the cell wall pathway as well as transport from cell to cell through their membranes.

Finally, Molz(1976) introduced a model which allows for the water flow through the apoplasm and the symplasm of the plant tissue for non diffusing solutes. Both are accepted pathways that a solvent or solute may follow.

The microscopic description of the mass transport phenomena in plant storage tissue seems to offer the greatest potential in modelling the mass transfer in vegetables and fruits upon osmotic dehydration. It has been put forward by plant physiologists and used to model the air dehydration of foodstuff with successful results.

More recently, Toupin(1986) developed a model on the mass transport phenomena in plant material based on the model presented by Molz et al.(1979). Diffusion of impermeable and permeable species in the matrix was considered as well as the shrinkage of the whole structure. The results obtained were satisfactory although many of the parameters of the cell and the tissue were estimated and adjusted because of the lack of experimental data. Very little work has been done on the measurements of the spatial distribution of the osmotic effect and the equilibrium parameters as compared to the drying process for example. Toupin(1986) showed, with sufficient evidence, that the transport of matter across biological membranes is properly dealt within the theory of thermodynamics of irreversible process and the permeability data of these membranes can be obtained. The model was compared satisfactorily with experimental measurements in terms of cell volume changes.

According to Toupin(1986), a cell can be simplified further in terms of mass transport due to osmosis (fig. 2.9). The cellular volume comprises the vacuole, the tonoplast, and the cytoplasm. The plasmalemma controls osmosis by its selective permeability and the extracellular volume includes the intercellular space and the cell wall.

Most of the problems of the model developed by Toupin arose in the description of the tissue behavior. First, some assumptions have been made in order to deal with the global structural changes of the tissue or shrinkage. Three stages of dehydration were assumed. In the first stage, the global change in volume is equal to the change in the cellular volume which comprises the cytoplasm, the tonoplast, and the vacuole. The second stage is characterized by a constant total volume of the tissue. The third stage is assumed in order to describe the shrinkage when there is collapse of the structure. The total change in volume is equal to the change in cellular volume. The introduction of the critical cell volume was made in order to take into account the third stage of dehydration which corresponds to the loss of the cell integrity. Second, the lack of equilibrium data describing the behavior of the tissue upon osmosis, similar to sorption data in drying, led to an improper description of the changes of the different phases of the cell, particularly the cellular volume. The apparent non osmotic volume was introduced to compensate.

The need for further studies in the area of internal mass transfers in a biological structure due to osmosis was felt from an experimental point of view as well as from a modelling point of view.

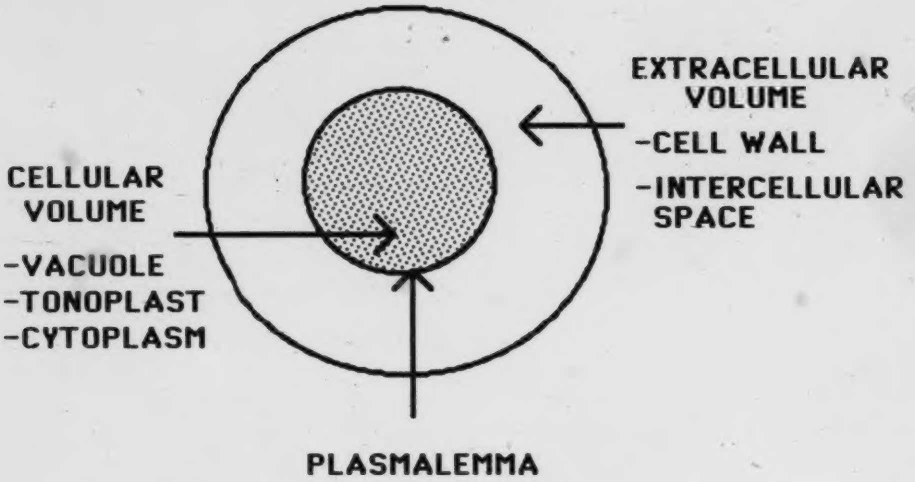

EXTRACELLULAR VOLUME
-CELL WALL
-INTERCELLULAR SPACE
CELLULAR VOLUME
-VACUOLE
-TONOPLAST
-CYTOPLASM
PLASMALEMMA

Fig. 2.9 Simplified Cell of Plant Material.

3. EXPERIMENTAL WORK

3.1 Materials

3.1.1 Selection of the solute

3.1.1.1 Advantages of Sucrose

Since the theory of irreversible processes describes fairly well the transmembrane transport, there was no need to complicate the system. Sucrose was chosen because of its impermeability to the cell membrane which brings the two following major consequences. The transmembrane transport is simply the flux of water through the membrane. It is proportional to the chemical potential of water. Secondly, the space available for the sucrose to move is restricted to the extracellular volume.

Furthermore, Lenart and Flink(1984b) pointed out the differences between osmosis in salt and sucrose solutions. Sucrose was found to be the more critical component in determining the osmotic behavior in salt/sucrose mixture. Sucrose osmosis appears to approach equilibrium primarly by removal of water from the tissue and, thus, to achieve equilibrium will require the removal of a significant amount of water as there is little solids uptake due to the membrane property of selective permeability. This is a characteristic of osmotic dehydration and conventional models are not able to describe the behavior properly. Salt penetrates readily into the potato tissue. The membrane does not seem to offer a significant resistance to the passage of the solute. The results for the distribution of solids gain and water loss for osmosis in salt indicates that there is an equality of sorts between the potato tissue and the osmotic solution. This type of behavior is more easily dealt with by conventional models such as the unsteady state second order Fickian equation. Thus, modelling of the osmotic behavior of a biological material in a sucrose solution is representative of the typical osmosis behavior leading to dehydration since the solute is strictly impermeable to the membrane.

3.1.1.2 Properties of Sucrose and Water in Solution

Since the major mass transfers involve sucrose and water, the solutions in the extracellular volume as well as in the osmoticum are assimilated to binary sucrose solutions. Partial molar volumes and molecular weights were obtained from standard tables(Weast et al., 1984) and are respectively for water and sucrose 18.016 x 10^{-3} and 211.0 x 10^{-3} m^3/mol for the partial molar volumes and 18.0 and 342.2 kg/mol for the molecular weights. Diffusion occurs in the extracellular volume. The nature of the concentration dependence of the diffusion coefficient of sucrose in water can be found experimentally. A fitting of the logarithm of the ratio of the standard diffusion coefficient over the standard diffusivity at infinite dilution as a function of the sucrose concentration was obtained from the experimental measurements (Landolt-Bornstein tables, 1969). A polynomial of degree 1 (i. e., a straight line relationship) was found adequate (r=0.9973) to describe the dependence leading to:

$$\ln \frac{D_s}{D_s^{\infty}} = a_0 + a_1 \rho_s \qquad [3.1]$$

where D_s is the standard diffusion coefficient of sucrose at a concentration ρ_s in water at 25°C, D_s^∞ is the diffusivity at infinite dilution at 25°C and is equal to 5.23×10^{-10} m^2/s. The coefficient a_0 is equal to zero. a_1, the coefficient of the polynomial of degree 1, is equal to -2.088×10^{-3} m^3/kg. Correlation was obtained with data at 25°C. Henrion(1964) has shown that the standard diffusivity is a unique function of concentration. The diffusivity at infinite dilution at 40°C was estimated by the relation $D_s\mu/T = 0.0157$ and found to be 7.53×10^{-10} m^2/s.

Solutions were prepared using commercial sugar bought from a local supermarket.

3.1.2 Selection of the Biological Structure

3.1.2.1 Guidelines

The tuber of potato was selected as a biological structure because of its relative homogeneity and firmness. The dicing or slicing may be done easily. The possibility of obtaining various geometrical shapes is almost unlimited. This type of material is also colorless which represents an advantage for the chemical analysis.

3.1.2.2 Physiological Parameters of the Potato

3.1.2.2.1 Chemical Composition of the Tuber

Different varieties of potatoes are available on the market. Russet Burbank cultivar is one of the older varieties. Because of its excellent cooking quality particularly for baking and frying, this variety is widely processed in the food industry. Furthermore, physiological parameters are relatively abundant in the literature.

Talburt, Schwimmer and Burr(1975) observed that although the literature on the chemistry of the potato is extensive, it is difficult to obtain a definite picture of the composition. Variety, area of growth, cultural practice, maturity at harvest, subsequent storage history etc... were found to contribute to variation between reported results. The methods of analysis were also observed to contribute to the variability of the reported results. Consequently, the analysis of white potatoes published by Talburt, Schwimmer and Burr(1975) and shown on table 3.1 must be regarded as only approximate and subject to all sources of variation mentioned above. It has to be pointed out that Russet Burbank variety is classified as a white potato but not exclusively. The water content ranges from 63.2%-86.9% with 77.5% on average. The total solids usually varies from 13.1%-36.8% with an average of 22.5%. Proteins constitute about 2% of the total weight of the potato. Fat content is negligible. Most of the solids are carbohydrates, particularly starch which comprises 65%-80% of the dry weight of potato. Ash is about 1% of the total weight of the tuber. The major minerals present in the potato tubers are listed in table 3.2. The ash content of a raw tuber is composed mainly of potassium, phosphorous, magnesium, calcium, and finally sodium in order of magnitude.

In Alberta, Russet Burbank potato tubers from the northern, the central, and the southern part were analyzed by Chung(1979) in terms of

Table 3.1 Proximate Analysis of White Potatoes.

Table 3.1 has been removed due to the unavailability of copyright permission.

Table 3.2 Composition of Ash[1] from White Potatoes on a Dry Ash Basis.

Table 3.2 has been removed due to the unavailability of copyright permission.

ash content, dry matter, and starch. It was found that more that 90% of the minerals were located outside the starch granules. The ash content of the raw tubers grown in the southern part of Alberta varied from 2.68%-3.35% on dry matter basis. It was observed to be lower than the mineral content of the tubers grown in the northern part of Alberta (4.72%-5.68%). Only 0.36% minerals were found in the starch as phosphorous. The dry matter ranged from 19.06%-26.06% from the northern to the southern part of Alberta. Finally, the starch content of the southern tubers was observed to be 76.06% whereas the northern ones contain 68.99% starch on a dry matter basis.

Crapiste and Rotstein (1982) published two distinct, limiting, simplified representative compositions of a raw potato tuber. These compositions reflect also the variation between the area of growth of the same variety as it was found by Chung(1979). Table 3.3 shows the different compositions reported by Crapiste and Rotstein(1982). They will be used for calculations and in the discussion of some of the results particularly the composition B.

3.1.2.2.2 Storage of the Potato Tubers and its Relationship to Total Solids Content, Specific Gravity, and Sugars Content

The storage of the potato tuber at temperature below 10°C has the following major consequence. Sweetening of the potato occurs i. e., increase of the level of reducing sugars (fig. 3.1) and sucrose. The magnitude is dependent upon the variety and the storage temperature.

The effect of storage on different parameters such as total solids, specific gravity, reducing sugars and sucrose has been studied by numerous authors.

Table 3.3 Simplified Representative Composition of the Dry Matter of the Potato Tissue.

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Fig. 3.1 has been removed due to the unavailability of copyright permission.

Fig. 3.1 Effect of Storage Temperature on the Reducing Sugars for Russet Burbank and Norgold Cultivar (Agle and Woodbury, 1968).

Habib and Brown(1959) found the Russet Burbank cultivar to undergo a slight increase in total solids and specific gravity upon storage and a major increase in reducing sugars. Before storage, the total solids content of raw potatoes was 22.28%. After storage at 4.4°C for 4 weeks the total solids content was found to be 23.10%. The specific gravity of raw potatoes was found to be 1.074 whereas after storage at 4.4°C for 4 weeks, it was 1.077.

Sayre et al.(1975) studied the variability in total solids content and specific gravity between tubers and also within the same tuber. Russet Burbank stored for 6 months at 7°C were used. They found that the average total solids content of 20 tubers was 20.5% within a range 17.5%-22.8%. The spread in solids content among samples from individual tubers was from 7 to 13 percentage points.

Agle and Woodbury(1968) examined the effect of storage on the percentage of dry matter and on specific gravity. A very slight increase in total solids was found.

Fig. 3.2 illustrates a typical linear relationship between the potato solids content and the specific gravity as is usually done in the literature.

Talburt, Schwimmer and Burr(1975) reported that White Rose and Russet Burbank varieties accumulate reducing sugars at storage below 10°C, the accumulation going through a maximum after about 4 weeks to 8 weeks then dropping to a relatively constant but high level (fig. 3.3). For poor sugar accumulators such as Russet Burbank the maximum sugar concentration reached may be as much as 3% on a dry weight basis.

A similar trend was observed by Agle and Woodbury(1968) and Zaehringer et al.(1966). Basically a rapid build-up of sugars, such as

Fig. 3.2 has been removed due to the unavailability of copyright permission.

Fig. 3.2 Regression Equation for Percent Dry Matter versus Specific Gravity for Russet Burbank Cultivar (Agle and Woodbury, 1968).

Fig. 3.3 has been removed due to the unavailability of copyright permission.

Fig. 3.3 Effect of Time in Storage at 5.5°C on the Reducing Sugars for Russet Burbank and Norgold Cultivar (Agle and Woodbury, 1968).

sucrose, glucose and fructose, early in the storage period followed by a slight decline or a plateau has been observed. As the temperature gets closer to the freezing point, the rate and extent of increase in sugar content is greater.

Finally, Iritani and Weller(1977) found that immature tubers have a higher sucrose and reducing sugars content than mature tubers.

Table 3.4 summarizes data reported in the literature on the sucrose, glucose and fructose content after different storage periods.

3.1.2.2.3 Structure of the Potato Cell

Parenchymatous cells, which compose the edible part of the potato, are the most common cell type in the tubers. The cells are large, polyhedrical or spherical in shape. Although Crapiste and Rotstein(1982) reported a cell diameter between 250-500μm, Reeves (1967) found that the average cell diameter of mature tubers (200-300g) for Russet Burbank cultivar varied between 192-213μm. In Alberta, Chung(1979) measured an average cell diameter of 180μm for Russet Burbank variety.

The potato tuber possess a single large vacuole which may occupy over 90% of the total cell volume. This vacuole is a relatively diluted homogeneous aqueous phase. It contains up to 80%-90% of the cell water. Minerals, sucrose, glucose, fructose, organic acids and vitamins contribute to the vacuole solution. The vacuole is known to be a storage reservoir for toxic products and metabolites (Nobel, 1983). The tonoplast separates the vacuole from the cytoplasm. The cytoplasm is a more complex phase containing many colloids and membrane bounded organelles (Nobel, 1983). Reserve materials such as starch and proteins

Table 3.4 Literature Survey of Sucrose, Glucose and Sucrose Content of Stored Potatoes (Russet Burbank Cultivar).

Authors	Storage Time (month)	Storage T (°C)	Reducing Sugars GL %FWB (%DWB)	Reducing Sugars FR	Sucrose %FWB (%DWB)
Wilson et al.(1981) (HPLC)	NA	3.3	0.8	0.68	0.26
	NA	7.2	0.16	0.077	0.065
Zaehringer*+ et al.(1966)	1-6	3.3	1.87 (8.9)		1.13 (5.4)
	1-6	7.2	0.38 (1.8)		0.27 (1.3)
	1-12	3.3	1.55 (7.4)		0.92 (4.4)
	1-12	7.2	0.40 (1.9)		0.25 (1.2)
Zaehringer*++ et al.(1966)	1-6	3.3	1.66 (7.9)		0.54 (2.6)
	1-6	7.2	0.32 (1.5)		0.21 (1.0)
	1-12	3.3	1.45 (6.9)		0.46 (2.2)
	1-12	7.2	0.29 (1.4)		0.14 (0.7)
Shallenberger and Treadway(1959)	2	0	0.74		2.01
	2	10	0.40		0.28
[illegible]bib and* Brown(1959)	1	4.4	0.27 (1.18)		

* Assumption 21% dry matter
+ 1963 crop
++ 1962 crop

are present in the cytoplasm. In the raw tuber, starch is present as microscopic granules in the leucoplasts lining the interior of the walls of the cells of the parenchyma tissue (Talburt, Schwimmer and Burr, 1975). Some 70%-80% of the extractable true protein belongs to so-called "storage protein" (Hadziyev and Steele, 1979). In constrast to which, the concentration of soluble solutes is very low.

A membrane separates the cell wall from the cytoplasm. The plasmalemma, which is the main barrier, regulates what enters and leaves a plant cell. As it was mentioned, the selective permeability of the plasmalemma membrane towards sucrose and water determines the osmotic behavior. The membrane is composed of a lipid bilayer. To form a bilayer, the lipid molecules (mainly phospholipids) have their non polar portions adjacent to each other facilitating hydrophobic interactions. The polar regions are then on the outside.

A membrane represents a different type of molecular environment than does an aqueous solution. The transport of species is greatly restricted compared with the relatively free movement in an aqueous phase. The relative solubility of a species in the two phases influences the membrane permeability property. Water and carbon dioxide readily penetrates the plasmalemma whereas sucrose is a non permeating solute. Rotstein and Cornish(1978a) found a certain degree of confusion in their literature survey as to the value of the water permeability constant which mostly depends on the driving force and the mathematical expressions chosen. They listed some values for vegetable cells. For Solanum tuberosum $\mathcal{P}_{wm}$ is equal to 14.4×10^{-6} m/s (Heinrich, 1962).

Because of the cell wall, high hydrostatic pressures can exist inside the cell. The cell wall provides the rigidity to allow for a build-up of pressure. The cell wall elastic modulus, ξ, of the potato cell was found to be pressure dependent. Referring to Nilsson et al.(1958), the variation of ξ with respect to the intracellular hydrostatic pressure was characterized by two parameters $\beta_1$and β_2:

$$\xi = \beta_1 P + \beta_2 \qquad [3.2]$$

where β_1 is taken as 3.5 and β_2, the value of ξ at incipient plasmolysis, is 0.5×10^6 Pa experimentally. P is the turgor pressure in excess to the atmospheric pressure.

According to Slatyer(1967), the cell wall of vegetables at full turgor contains about 50% water on a volume basis. The void fraction of the cell wall (ϵ_{cw}) is thus 0.5. Cellulose comprises 25% to 50% of the cell wall organic material of the potato tuber. Hoff and Castro(1969) described the cell wall composition of the potato tuber on a dry matter basis as follow: 28% cellulose, 55%-66% pectins, 7% hemicellulose, 10% proteins. The tortuosity of the cellulosic matrix (τ_{cw}) is assumed to be 2.0 (Nobel, 1983). Nobel(1983) reported that the cell wall for plant tissue may vary from 0.1 to 10μm. Reeves et al.(1973a) found that the cell wall of the potato tuber was 1.05μm thick which was confirmed by a transmission electron micrograph done by Chung(1979).

Cells of potato tubers are closely packed but there is a certain amount of intercellular space. Woolley(1962) found the intercellular spaces to be interconnecting and air filled except at the cut surface, where most spaces were water filled to a depth of a few microns. There is a lot of variation in the literature for values of the proportion of the intercellular space of the potato tissue. Burton and Spragg(1950) published a value of 1% intercellular space for potato tissue. However, the same authors also reported other literature values varying from 2.0%-3.4% intercellular space for different varieties of potatoes. Davis(1962) noticed a decrease of the air space upon storage, the average being shifted from 1.45% to 1.14% air volume. He also reported other literature values. Finally, Crapiste and Rotstein(1982) assumed a fraction of intercellular space, of 1% to 3% at full turgor. The microscopic observations indicate that the cell wall and intercellular space of many tissue constitute 7 to 10% of the total volume (Salisbury and Ross, 1969). Assuming that the intercellular space volume fraction is 3% the cell wall volume fraction would be approximately 5% of the total tissue volume. However, using the measurement of the cell wall thickness (1.05μm) and the diameter of the cell (180μm), the volume fraction of the cell wall would be 1.7%.

Today, it is generally accepted that most plant cells are joined to each other by protoplasmic connecting treads. The presence of plasmodesmata as well as their frequency is related to a functional role which is to provide an alternative transport pathway of least resistance for water and solute to travel along. Tyree(1970) pointed out that the ratio between the water permeability of the plasmodesma pseudo-membrane ($\mathcal{P}_{wp}$) would be at least two orders of magnitude higher that the water permeability of the plasmalemma, $\mathcal{P}_{wm}$, (Anderson, 1976). The symplasm transfer area of higher plant cells is reported by Ferrier and Dainty(1977) to occupy 1% of the plasmalemma area. The conclusions of Robards(1976) show that this fraction does not exceed that limit in higher plants.

For this experimental work, Russet Burbank cultivars grown in Northern Alberta were used. They were kindly provided by I. & S. Produce Ltd, a local food processor. Freshly bought potatoes (Russet Burbank cultivar) were divided into groups according to their weight: first group, below 200g; second group, 200g-300g; third group, over 300g. All experiments were conducted using tubers from the second group in order to avoid variability due to maturity and to ensure a sufficient amount of potato material. The potato tubers were stored at 4°C at least a month prior to the osmotic treatment. The storage time and temperature influence considerably the sugar content such as glucose, fructose, and sucrose. Consequently, they have a significant impact on further experiment involving an osmotic water removal process in a sucrose solution. Standardization of storage time and temperature is necessary in order to achieve some consistency in the experimental results. Furthermore, experiments were conducted on potatoes stored at 4°C for at least 2 months but less that 6 months so that the sucrose content was high but constant.

3.2 Methods

3.2.1 Equilibrium Study

3.2.1.1 Conditionning of the Potato Tissue

Potato tubers (10) were selected from the cold room and were used to obtain 280 disks of parenchyma tissue. A few cores were cut from the tubers using a cork borer (size 14). These cylinders were sliced using a sharp blade. The resulting disks (22mm diameter, 5mm thickness) were soaked in distilled water for at least 20 hours at 4°C prior to the osmotic treatment.

3.2.1.2 Sample Treatment

Solutions of the following sucrose concentrations (10%, 20%, 30%, 40%, 60% (w/w)) were prepared in triplicate by blending an amount of sucrose with distilled water on a weight to weight basis.

An osmotic experiment was conducted in the following manner: 18 slices were selected, blotted, weighed together accurately (m_{po}) (approximately 35g), and finally added to a vessel containing 500ml of an osmotic solution measured with a volumetric flask. Gentle agitation was provided by a magnetic stirrer and the temperature of the vessel was maintained at 40°C in a water bath for 24 hours. To prevent evaporation during the treatment a plastic wrap was put on top of the vessel. The diagram of the osmotic treatment apparatus is shown on fig. 3.4.

At the end of the osmosis period, the slices were rinsed quickly in five different beakers containing distilled water and gently blotted with paper in order to remove the surface solution.

The material was weighed again (m_{po}) to calculate the mass loss (ML) or weight loss. Immediately the slices were divided in three sets of six slices. Each set was used for three replicates (2 slices each) of either moisture content measurement or density determination or sugar content and insoluble solids measurements.

3.2.1.3 Measurement of Moisture Content

Moisture content was determined gravimetrically by air drying at 105°C for a 24 hour period.

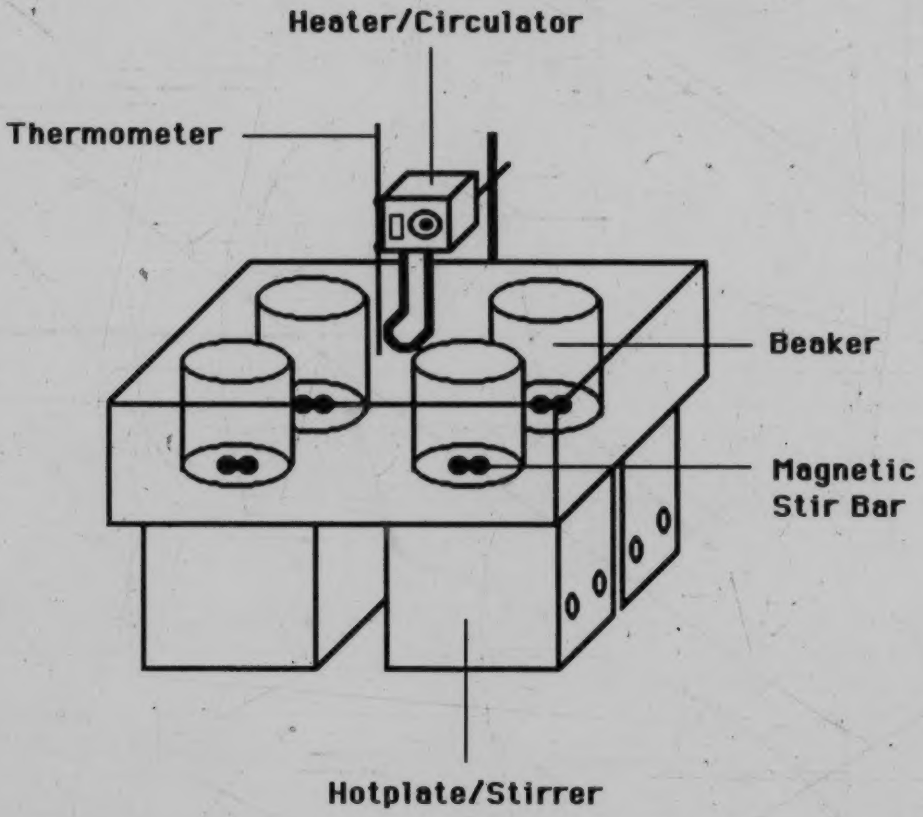
Heater/Circulator
Thermometer
Beaker
Magnetic Stir Bar
Hotplate/Stirrer

Fig. 3.4 Diagram of the Osmotic Treatment Apparatus for the Equilibrium Study.

Two slices were transferred to a preweighed aluminium dish, weighed and dried in the oven. After cooling in a dessicator under vacuum, the dish was reweighed and the moisture content was calculated.

3.2.1.4 Density Determination

The volume displacement technique was used in order to determine the density. Weight and volume were measured by weighing two disks in a preweighed empty pycnometer, filling up with water and reweighing. From the weight of the empty pycnometer and the volume of the pycnometer, predetermined by weighing the pycnometer filled with water at 23°C, the weight, the volume, and subsequently the density of the disks were calculated.

3.2.1.5 Measurement of Sucrose Content

3.2.1.5.1 LC System

The HPLC system consisted of a Bio-Rad model 1330 pump and a Waters Associates model R401 differential refractometer (RI) detector. The system was equipped with a 20μl Rheodyne loop injector. A Bio-Rad Aminex HPX-87H ion exclusion column (300 X 7.8mm i. d.) was used for the separation of sugars; the column being protected by a 40 X 4.6mm guard column. Quantitation was performed electronically with a Hewlett-Packard 3388A integrator.

3.2.1.5.2 LC Separation Conditions

The mobil phase used was 0.01N H_2SO_4. The solution was prepared using an analytical grade sulfuric acid obtained from Fisher Scientific and LC-grade water which was prepared by reverse osmosis (Milli-RO) and further purified by using a (Milli-Q) system (Millipore, Bedford, MA). After degassing, the mobil phase was used for LC analysis with a flowrate of 0.8ml/min at ambient temperature. Standard solutions of mixtures of analytical grade sugars (fructose, glucose and sucrose) ranging from 1-10mg/ml were run into the system.

3.2.1.5.3 Extraction and Measurement of Soluble Sugars

Potato slices (approximately 4g or 2 disks) were crushed with a mortar and pestle. The grindings were placed into a preweighed 50ml centrifuge tube and weighed prior to homogenization.

Extraction of sucrose, glucose and fructose was achieved by boiling the sample with double the volume of 80% ethanol for 15 minutes. Supernatant was poured off and vacuum filtered through a preweighed Whatman #4 filter paper with a Buchner funnel.

A fresh volume of 80% ethanol was added to the grindings for a second 15 minute extraction. The extract and the residue were poured off and vacuum filtered. The residue was well washed with 80% ethanol. The filtrate was made up to volume with distilled water either in a 200ml volumetric flask (for osmotic treatment with a 60% sucrose solution) or in a 100ml volumetric flask (for osmotic treatment with 10-40% sucrose solution). A certain volume of this extraction solution was filtered through a 0.45μm millipore membrane and an aliquot was injected into the HPLC system for the quantitation of sugars.

3.2.1.5.4 Measurement of Insoluble Solids

The residue of the extraction was transferred with the filter paper from the Buchner funnel into a preweighed aluminium dish to be air dried in the oven at 105°C for 24 hours. After cooling in a dessicator under vacuum the dish was reweighed and the insoluble solids (IS) content was calculated.

3.2.2 Kinetic Study

Three concentrations of osmotic solution were investigated for the kinetic study: 20%, 40%, 60% (w/w) sucrose solutions. The osmotic treatment was conducted over several time duration i. e. 1, 6, 24 hours. For each combination of time duration and concentration, six vessels were prepared and three mature tubers were selected from the cold room.

The osmotic solution was prepared by blending the sugar and distilled water on a weight to weight basis. 500ml of the osmotic solution was measured with a volumetric flask and poured into a 1000ml beaker. It has to be pointed out that two of these vessels containing the osmotic medium were set aside and were used subsequently for the determination of the sucrose uptake using an isotope dilution method.

Each potato was prepared for the treatment in the following manner: the potato tuber was coated with a thin layer of paraffin wax and then cut cross-sectionally into halves. Only the cut surface was available for the mass transport. The cutting was done while the wax was still warm, but cool enough to handle, in order to avoid cracking along the cut edge.

3.2.2.1 Sample Treatment

Each half was suspended in a vessel so that the free surface was approximately 5mm below the solution surface. Gentle agitation was provided by a magnetic stirrer and the system was maintained at 40°C in a constant temperature water bath for the duration of the treatment. In order to prevent evaporation the beakers were covered with a sheet of plastic wrap during the experiment. The set up of the experiment is shown on fig. 3.5

At the end of the osmosis period, the potato half was removed from the solution. Its surface was rinsed three times with water and gently blotted. The sample was set face down on a sheet of plastic wrap. A few cores (2, 3, 4 of 1.4 x 10^{-2} m diameter) were taken from each potato half using a sharp tubular cork borer (size 8). They were cut at right angle to the treated surface. Starting from the osmosed surface, each core was sliced into 10 disks (approximately 1.0 x 10^{-3} m thickness) with a modified microtome shown on fig. 3.6. The slices of each core were identified by their order of slicing. The summary of the osmotic treatment and sample preparation procedure is shown on the fig. 3.7 for each combination concentration of the solution, time duration.

In order to achieve reliable measurements on the density and moisture content, at least three or four slices were needed (approximately 0.8-1.0g of material) for each determination. The slices of the cores of the same potato half were matched according to the order of slicing, prior to the density and moisture content determination.

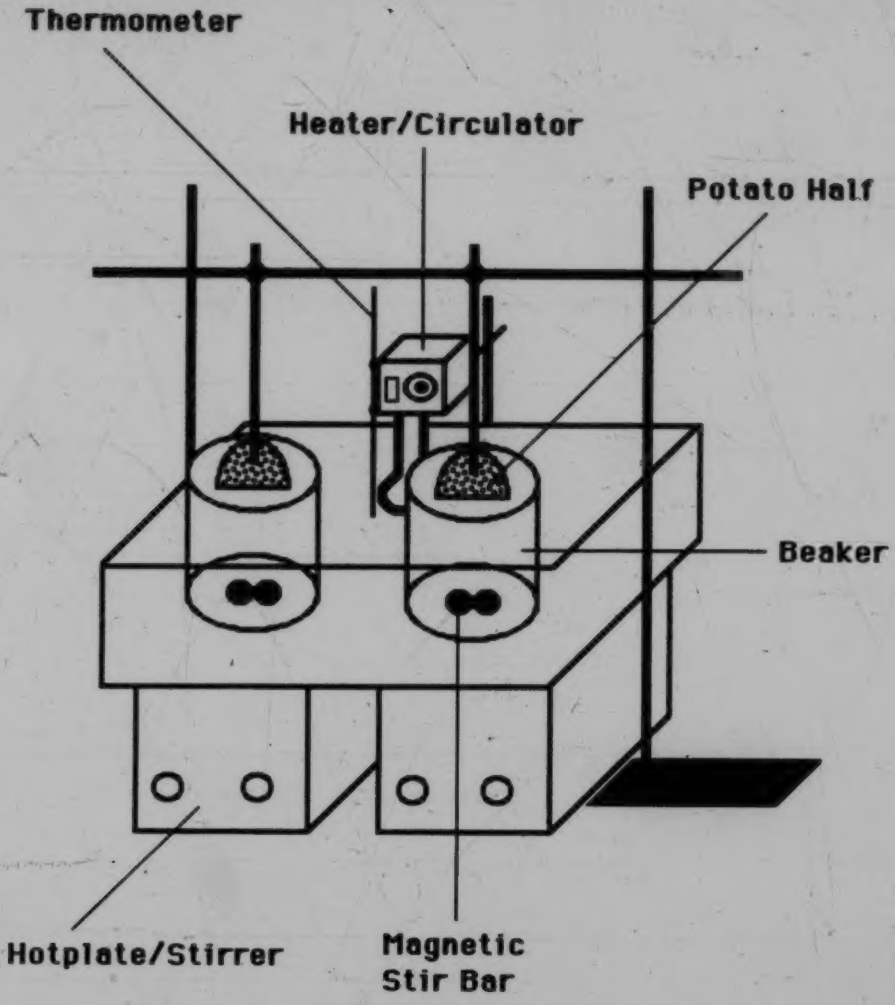
Thermometer
Heater/Circulator
Potato Half
Beaker
Hotplate/Stirrer
Magnetic
Stir Bar

Fig. 3.5 Setup of the Osmotic Treatment for the Kinetic Study.

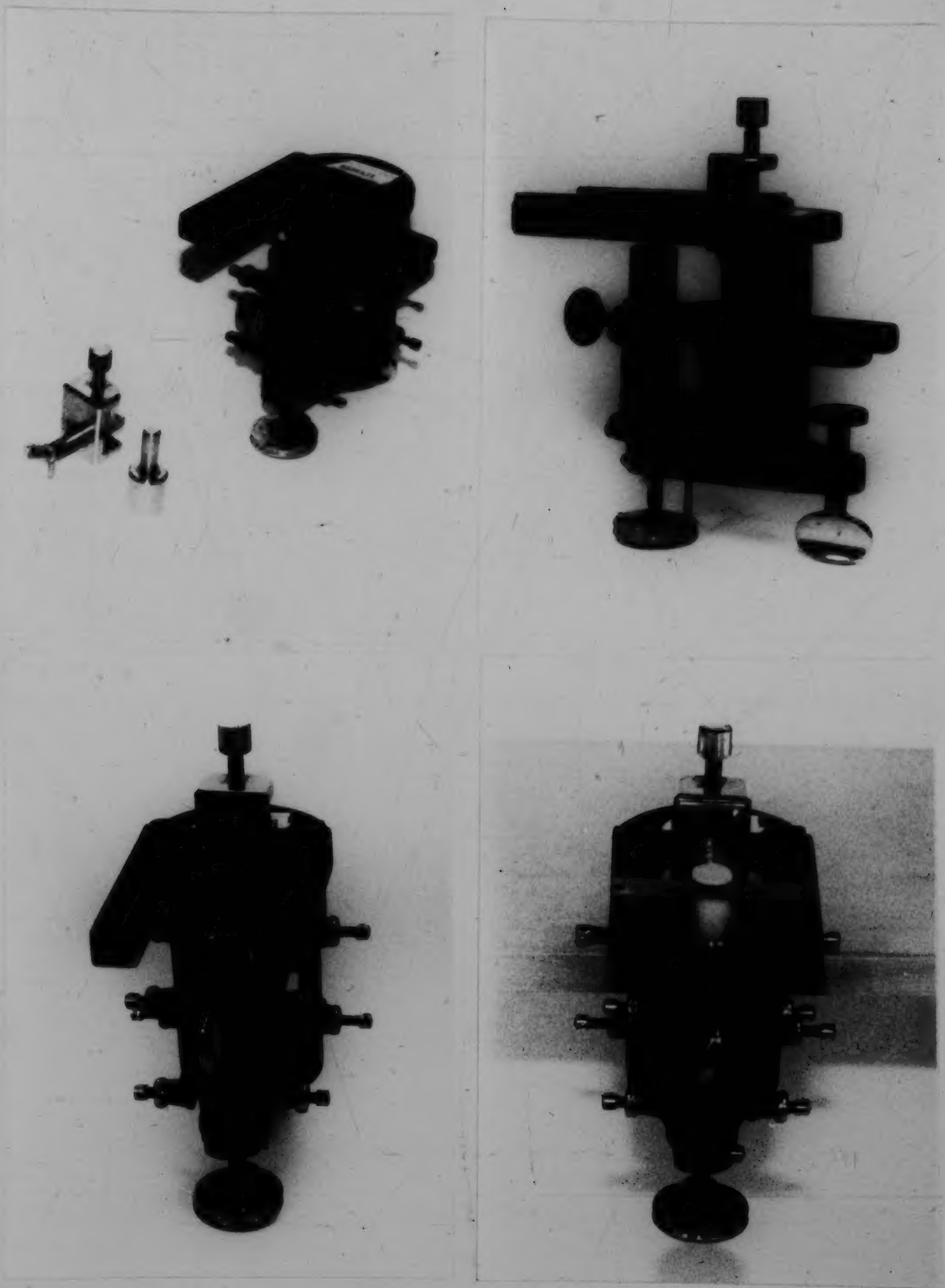

Fig. 3.6 Modified Microtome.

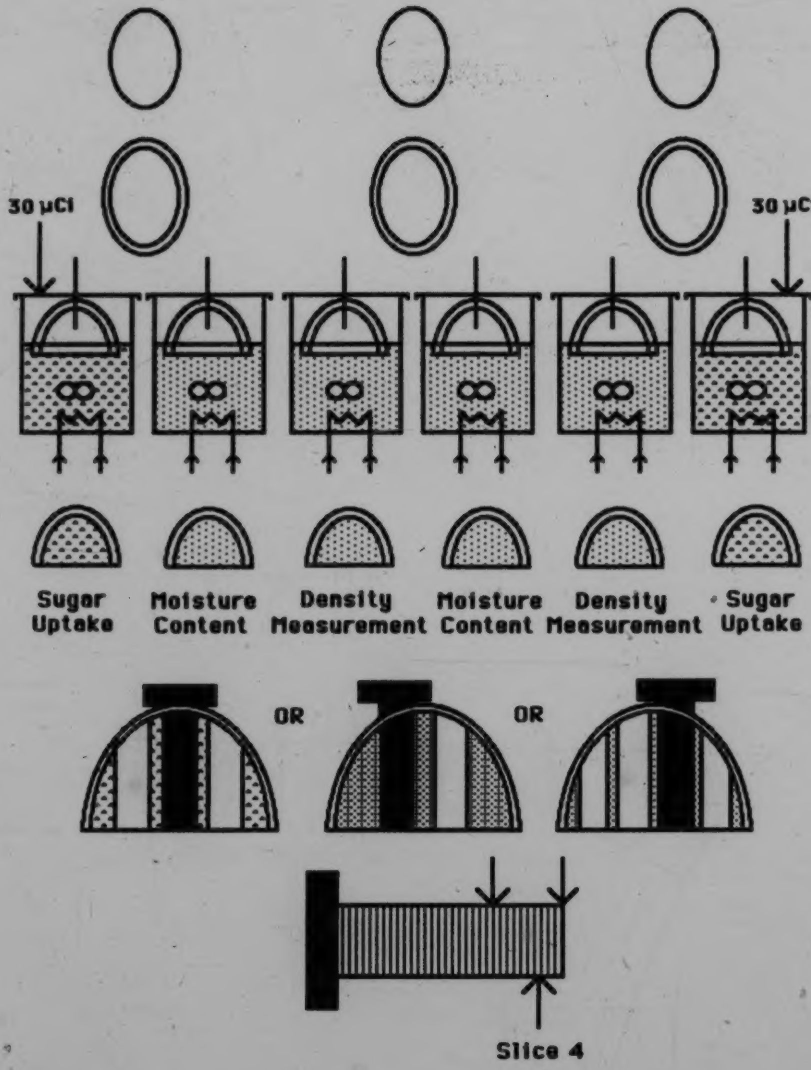
30 µCi
30 µCi
Sugar Uptake
Moisture Content
Density Measurement
Moisture Content
Density Measurement
Sugar Uptake
OR
OR
Slice 4

Fig. 3.7 Summary of the Osmotic Treatment and Sample Preparation Procedure for each Combination Solution Concentration, Time Duration of the Kinetic Experiment.

3.2.2.2. Measurement of Moisture Content

Moisture content of the potato was determined using the method described in section 3.2.1.3. Each of the 10 sets of slices (3 or 4 coming from the cores of the same potato half) was weighed before and after drying to calculate its moisture content.

3.2.2.3 Density Determination

The density determination of the potato slices was done using the technique described in section 3.2.1.4. Each of the 10 sets of slices (3 or 4 coming from the same potato half) were weighed in the preweighed pycnometers. Water at 23°C was added and the pycnometers reweighed. Knowing the mass of the pycnometer and the volume of the pycnometer, which was determined using water at 23°C, it is possible to calculate the density of the potato slices.

3.2.2.4. Measurement of Sucrose Uptake

3.2.2.4.1 Chemicals and Osmotic Treatment

In order to measure sugar uptake, radioactive sucrose was used as a tracer. The radiolabeled compound [U - ^{14}C] sucrose (250mCi/mmol) was purchased from Amersham (Arlington Heights, IL) as well as the ACS (Aqueous Counting Scintillant). Domestic bleach was obtained in a local supermarket and ammonium hydroxide from Fisher Scientific.

A measured quantity of labeled sucrose (30μCi) was added to the vessels of osmotic solution, previously set aside for this purpose, (section 3.2.2) prior to the osmotic treatment and sample preparation.

3.2.2.4.2 Tissue Preparation

After the osmotic treatment and sample preparation was carried out as described in section 3.2.2.1., each slice of radioactively osmosed potato (approximately 1.0 x 10^{-3} m thickness) was put in an empty preweighed liquid scintillation vial and weighed.

Prior to scintillation counting, the tissue was treated as described by Smith and Lang (1987). To each vial, 1ml of sodium hypochlorite (40%(v/v) domestic bleach) was added. The vials were loosely capped and incubated at 55°C for at least 4 hours. After bleaching, the digests were treated with 0.1ml NH_4OH 4M at room temperature for 1-2 hours in order to prevent sodium hypochlorite chemiluminescence. Before counting, 10ml of scintillation cocktail (ACS) was added to each vial.

3.2.2.4.3 Counting of the ^{14}C Labelled Sucrose

Samples were counted with a Beckman model LS 1801 scintillation counter. The data were obtained as desintegrations per minutes (dpm), by using a series of ^{14}C standards (kindly provided by the Department of Animal Science, University of Alberta) to generate a quench curve relating the instrumental counting efficiency to H number as specified by the manufacturer. Potato samples and samples of the osmotic solution before and after the osmotic treatment were counted.

The ratio of radioactive and ordinary sucrose remaining unchanged irrespective of the physical process that the sample undergoes, it is possible to calculate the amount of ordinary sucrose taken by the slice knowing the measured quantity of radioactive sucrose in the slice.

3.3 Results and Discussion

3.3.1 Equilibrium Study

The objective of the equilibrium study was to monitor the weight and volume changes of the potato i. e. the shrinkage of the whole tissue as a function of the sucrose concentration of the osmotic medium as well to determine the limiting composition of the potato material in different sucrose concentration of osmotic media.

3.3.1.1 Experimental Equilibrium Parameters of Potato Tissue as a Function of the Sucrose Concentration of the Osmotic Solution

The experimental measurements of the density (ρ), the total solids (TS), the sugar content (SC), the insoluble solids (IS) are listed in table 3.5. The reader is referred to the appendix 1 for details on the calculations of these measurements.

Potato slices were conditioned prior to any osmotic treatment i. e., the cells were at full turgor. Data of total solids and density measurements were treated statiscally using an anova test followed by a Duncan Multiple Range test (DMRT). The reader is referred to appendix 2 for details. The data for total solids and density of samples untreated and treated in a 5% osmotic solution seems to indicate that there is equilibrium between the fresh potato material and the osmosed samples. From the table 3.5, it can be seen that there is no significant difference between the density of the fresh material, the density of the potato soaked in a 5% sucrose solution as well as the density of the slices after a treatment in a 10% osmotic solution at 1% level. For $\alpha = 0.05$, there is no significant difference between the density of the

Table 3.5 Experimental Measurements of Density (ρ), Total Solids (TS), Sugar Content (SC) and Insoluble Solids (IS) of Potato Slices in Equilibrium with an Osmotic Solution at 40°C.

	Sucrose Solution (%)	Density (ρ) (g/cm^3)	Total Solids (TS) (%)	Sugar Content (SC) (%)	Insoluble Solids (IS) (%)
1	Blank****	1.058±0.006*	15±1*	≅0.23	13±2
2	Fresh	1.09±0.01	21±1	≅0.3++	NA
3	5	1.08±0.02	19±3*	NA	NA
4	10	1.098±0.006**	26±2**	4.6±0.4	19±4
5	20	1.132±0.009	32±1	10±1	19±1
6	30	1.171±0.004**	39.6±0.9**	17±4***	19±1
7	40	1.21±0.01	45.8±0.7	23.5±0.2	20±1
8	60	1.31±0.01	65.3±0.6	33.8±0.8	24±1

Average of 9 replicates for density and total solids measurements unless specified.
Average of 3 replicates for sugar content determination unless specified.

* Average of 8 replicates.
** Average of 6 replicates.
*** Average of 2 replicates.
**** Blank is the full turgor tissue after soaking in distilled water for at least 20 hours prior to any treatment.
++ From the literature.

DMRT

```
α = 0.01    1 3 2 4 5 6 7 8   1 3 2 4 5 6 7 8
              ___               ___
                ___

α = 0.05    1 3 2 4 5 6 7 8   1 2 3 4 5 6 7 8
                ___             ___
```

N. B. A line typed under any sequence indicates no significant difference at a given percent level.

fresh material and the potato slices soaked in a 10% osmotic solution. However, statistically only the total solids of the material in a 5% osmotic treatment and the fresh material are not significantly different for both confidence levels. Similar experimental results for total solids have been observed by Lenart and Flink(1984a).

The insoluble solids (IS) were found to be statistically constant for any treatment. Lenart and Flink(1984a) have always made this assumption. The insoluble solids remaining constant allows the following statement to be made: there was no leakage from the cellular volume, consequently, the cells were not destroyed. This supports the fact that the osmotic water-removal process is usually considered as a mild treatment compared to any other conventional drying operation.

Based on the experimental measurements, the following equilibrium parameters have been calculated: mass loss (ML) water loss (WL), sugar gain (SG) and insoluble solids loss (ISL).

As described by Lenart and Flink(1984a) the mass loss (ML) or weight loss can be defined as the net loss in weight by the potato material on an initial potato weight basis:

$$ML = \frac{m_{po} - m^{o}_{po}}{m^{o}_{po}} \times 100 \qquad [3.3]$$

The water loss is defined as the net loss of water from a potato on an initial potato weight basis. It was calculated from the mass loss (ML), the total solids of the potato material at full turgor (TS^{o}) and the total solids of the potato material after the osmotic treatment (TS):

$$WL = \left[\left[\frac{ML}{100} + 1\right]\left[1 - \frac{TS}{100}\right] - \left[1 - \frac{TS^{o}}{100}\right]\right] \times 100 \qquad [3.4]$$

The insoluble solids loss(ISL) was determined as the difference between the measured insoluble solids after the treatment (IS) and the insoluble solids at full turgor (IS^{o}) based on an initial potato weight:

$$ISL = IS\left[\frac{ML}{100} + 1\right] - IS^{o} \qquad [3.5]$$

The sugar gain (SG) is defined as the net uptake of sucrose by the potato material based on the initial weight of potato. It is a function of the mass loss (ML) and the sugar content of the material after the treament (SC):

$$SG = SC\left[\frac{ML}{100} + 1\right] \qquad [3.6]$$

Assuming that there is no loss from the cell except the water and only sucrose is gained, it is possible to calculate the sugar gain indirectly by difference (SGD) using an equation similar to the one developed by Lenart and Flink(1984a):

$$SGD = \left[\frac{ML}{100} + 1\right] TS - TS^{o} \qquad [3.7]$$

These parameters are reported in table 3.6 with the statistical analysis and plotted against the sucrose concentration of the solution on fig. 3.8.

Data of mass loss (ML) were statiscally treated using and anova test followed by a Duncan Multiple Range Test (DMRT). The reader is referred to appendix 2 for details. From table 3.6, the mass loss profile appears to go through a minimum value of approximately 28% at around 30%-40% sucrose solution. Among the treatments, only the treatment in a 60% sucrose solution was found to be significantly different from the others at 5% level. The mass loss of the potato tissue with a 20% sucrose solution is greater than with a 40% sugar solution. From a dehydration point of view, at equilibrium, there is no advantage to operate with a 40% osmotic solution but, most of the processes do not proceed until equilibrium is reached. Therefore, highly concentrated solutions such as 40% osmotic solution are recommended (Hawkes and Flink, 1978; Lenart and Flink, 1984a). A greater difference in chemical potential is generated under these conditions which allows for a faster water removal. However, the optimization of the solution in terms of concentration and composition remains an important aspect of an osmotic treatment in order to minimize the cost of the solute, the solute gain, and the time of the osmotic treatment as well as to maximize the mass and water loss. The equilibrium data of mass loss show that there is an optimum and the behavior of the tissue under different concentration of osmotic solution is not proportional to the concentration of the solution.

The statistical analysis of the water loss, insoluble solids loss, sugar gain and sugar gain by difference was performed using a Duncan

Table 3.6 Equilibrium Calculated Parameters i. e. Mass Loss (ML), Water Loss (WL), Insoluble Solids Loss (ISL), Sugar Gain (SG), and Sugar Gain by Difference (SGD) of the Potato Slices in Equilibrium with an Osmotic Solution at 40°C.

	Sucrose Solution (%)	Mass Loss (ML) (%)	Water Loss (WL) (%)	Insoluble Solids Loss (ISL) (%)	Sugar Gain (SG) (%)	Sugar by Difference (SGD) (%)
1	5	-30±2	-28±2	NA	NA	-2±2
2	10	-32.6±0.8	-35±2	0±5	3.1±0.3	2.5±0.4
3	20	-30.5±0.6	-38±4	0±3	7.0±0.8	7.2±0.8
4	30	-28.4±0.6	-42±5	1±3	12±3	13±1
5	40	-28±1	-46±5	1±3	16.9±0.4	18±2
6	60	-46±1	-66±6	0±3	18.3±0.8	20±2

DMRT

DMRT																										
α = 0.05	5	4	1	3	2	6	2	3	4	5	6	2	3	4	5	6	2	3	4	5	6	2	3	4	5	6
				—	—			—	—	—		—	—	—	—	—				—	—				—	—
	—	—	—	—			—	—	—																	

Comparison of the mean sugar gain (SG) and the mean sugar gain by difference (SGD) for an osmotic solution shows:

α = 0.05	SG1	SGD1	SG2	SGD2	SG3	SGD3	SG4	SGD4	SG5	SGD5
	—	—	—	—	—	—	—	—	—	—

N. B. A line typed under any sequence of means indicates no significant difference at the given percent level.

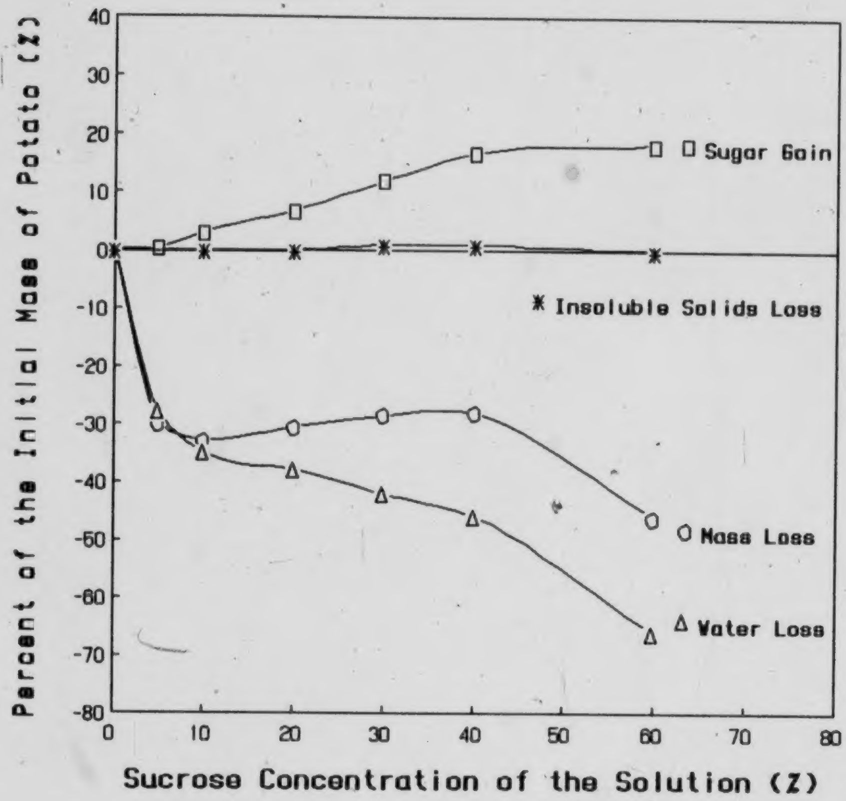

Fig. 3.8 Experimental Equilibrium Parameters.

Multiple Range Test. The error on the means were obtained by propagation of the error on experimental measurements. The reader is referred to appendix 3 for details. The water loss during an osmotic treatment varies from 28%-66% for a range of 10%-60% sucrose solution. Data from table 3.6 indicate that the water losses are not statistically different for the 10%, 20%, 30% and 20%, 30%, 40% osmotic treatments.

From fig. 3.8, it can be seen that sugar gain is not negligible. Among the five treatments there was no significant difference in sugar gain between an osmotic treatment in a 40% and in a 60% sucrose solution. The rate of sugar gain seems to decrease.

On table 3.6 the results show that direct measurements of sucrose are not significantly different from the sugar gain by difference calculated by eq.[3.7]. It seems to indicate that the method for the analysis of sucrose is good as well as to indicate that the main and only significant exchanges were sucrose and water within the experimental error.

The final amount of water loss (WL) and sugar gain (SG) were similar to those observed by Lenart and Flink(1984a).

3.3.1.2 Experimental Total, Extracellular and Cellular Volumes as a Function of the Sucrose Concentration of the Osmotic Solution

Data have been transformed in order to show the separate behavior of the total volume (V), the extracellular volume (V_i), and the cellular volume (V_c). The following assumptions have been used in order to proceed: sucrose as an impermeable solute is only present in the intercellular space and the cell wall. The liquid phase of the interstitum or extracellular space is at the same concentration as the concentration of the osmotic solution. In other words, there is saturation of the liquid phase of the extracellular space of the tissue.

The experimental total volumes were calculated from the mass loss (ML) and the density of the potato tissue at full turgor (ρ^o) and after the osmotic treatment (ρ). The proportion of total volume based on the initial volume at full turgor is determined by:

$$\frac{V}{V^o} = \left(1 + \frac{ML}{100}\right) \times \frac{\rho^o}{\rho} \qquad [3.8]$$

From the sucrose content measurements (SC) the proportion of volume of the extracellular space can be calculated based on the initial volume at full turgor.

$$\frac{V_i}{V^o} = \frac{SC\left[1 + \frac{ML}{100}\right]}{\rho_s} \times \rho^o \times \frac{1000}{100} \qquad [3.9]$$

ρ_s is the volumetric mass of sugar for a particular solution:

Solution	ρ_s
10%	103.8g/l
20%	216.2g/l
30%	338.1g/l
40%	470.6g/l
60%	771.9g/l

By difference the cellular volume as a proportion of the intial total volume is calculated:

$$\frac{V_c}{V^o} = \frac{V - V_i}{V^o} \qquad [3.10]$$

The reader is referred to appendix 3 for details on the statistical analysis of the volume changes. The total volume ratio plotted against the concentration of the osmotic solution on fig. 3.9 gives an initially straight, slopping line which bends sharply to the horizontal for a wide range of concentration and continues to decrease. From table 3.7, it can be seen that for osmosis in a 10%, 20%, 30%, 40% sucrose solution, the total volume of the tissue is statistically constant.

Fig. 3.9 shows that the extracellular volume ratio (V_i/V^o) is constant from 0 to ≈ 10% sucrose solution where the extracellular space increases sharply and then slightly.

The cellular volume ratio (V_c/V^o) of the tissue decreases. Since the loss of water can only come from the cellular volume i. e. sucrose is impermeable to the plasmalemma membrane, this type of profile is expected.

3.3.1.3 **Characteristic of the Calculated Equilibrium Parameters of the Potato Cell as a Basic Unit of the Potato Tissue**

The design, modelling, and optimization of any food process such as drying, packaging, or osmotic water removal process, require the equilibrium relationship which represents the moisture content of the food with respect to the temperature and the humidity of its environment.

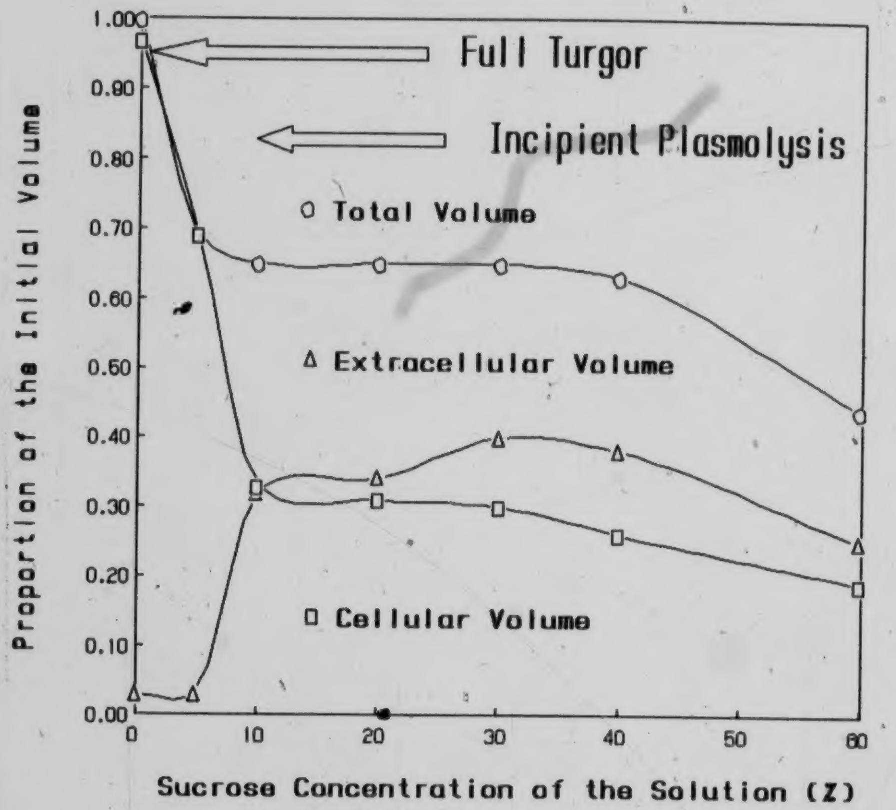

Fig. 3.9. Volume Changes based on Experimental Measurements.

Table 3.7 Experimental Volumes of Potato Slices in Equilibrium with an Osmotic Solution at 40°C.

	Sucrose Solution (%)	Total Volume V/V_o	Extracellular Volume V_i/V_o	Cellular Volume V_c/V_o
	Blank	1.0	0.047*	0.953
1	5	0.69±0.03	≅0.047**	0.69±0.03
2	10	0.65±0.02	0.32±0.03	0.33±0.05
3	20	0.65±0.02	0.34±0.04	0.31±0.06
4	30	0.65±0.02	0.4±0.1	0.3±0.1
5	40	0.63±0.03	0.38±0.01	0.26±0.04
6	60	0.44±0.02	0.25±0.01	0.19±0.02

DMRT

$\alpha = 0.05$ $1\ \underline{2\ 3\ 4\ 5\ 6}$ $1\ \underline{2\ 3\ 4\ 5\ 6}$ $1\ \underline{2\ 3\ 4\ 5\ 6}$

*Crapiste and Rotstein(1982).
** Since the sucrose gain was negligible.

In conventional drying operations, sorptional equilibrium isotherms are commonly used and readily available for these purposes. Crapiste and Rotstein(1982) published a correlation for the prediction of sorptional equilibrium of potato tissue from turgor to bonedry taking into account the structure and chemical composition of the cell as a basic unit of the tissue. The proposed method for water accounting in the biological structure is based on the fact that chemical potential is the most suitable parameter describing the state of water in any system particularly the equilibrium state of a multiphase system such as a plant cell with the environment. Restricting the treatment to non-electrolytes with the reference state of pure water at the temperature under consideration and atmospheric pressure, the water chemical potential of a vegetable system:

$$\mu_w - \mu_w^o = \mathbb{R}T \ln \hat{a}_w + \bar{V}_w\varphi_m + \bar{V}_w(P - P^o) \qquad [3.11]$$

The energy state of water is split into three major components. The first term ($\mathbb{R}T \ln \hat{a}_w$) reflects the contribution of dissolved solutes to the chemical potential of water or osmotic potential. $\bar{V}_w\varphi_m$ arises because of strong interactions between water and solids and large area of interface present in the system or matric potential and the final term, $\bar{V}_w(P - P^o)$, expresses the dependence of the chemical potential on hydrostatic pressure. This thermodynamic approach is widely used to describe the water relations of plant cells.

Considering the vegetable system in equilibrium with moist air, assuming an ideal gas behavior which is acceptable at atmospheric pressure:

$$\mu_w - \mu_w^o = \mathbb{R}T \ln \Psi \qquad [3.12]$$

Considering the vegetable system in equilibrium with an osmotic solution:

$$\mu_w - \mu_w^o = \mathbb{R}T \ln \hat{a}_{wos} \qquad [3.13]$$

Combining eq.[3.12] and eq.[3.13]:

$$\Psi = \hat{a}_{wos} \qquad [3.14]$$

The freezing point depression (FPD) of the solutions allows for the calculation of the water activity for each of the osmotic solution by the following equation (Wall,1974).

$$-\log \hat{a}_{wos} = 4.209\text{x}10^{-3}(\text{FPD}) + 0.215\text{x}10^{-5}(\text{FPD})^2 \qquad [3.15]$$

which has to be corrected for the temperature:

$$\ln \frac{\hat{a}_{wos}^{T}}{\hat{a}_{wos}^{To}} = 0.010146\, m_s^2 \ln \frac{T}{To} \qquad [3.16]$$

where m_s is the molality of sucrose solution, To is the freezing temperature, T is the temperature at which the water activity ($\hat{a}^{T}_{wos}$) is required and $\hat{a}^{To}_{wos}$ is the water activity at the freezing point depression temperature (To). The reader is referred to appendix 4 for details. The results are listed in table 3.8 for each sucrose concentration of osmotic solutions.

A typical composition of the potato tissue is required in order to assign the proper weight of the contribution of the different phases of in the potato tissue. Table 3.9 reports the average composition of the potato tissue which was found to agree with the composition of the potato tubers (Russet Burbank variety from the northern part of Alberta) selected for the experimental work. Considering that the tissue structure is made up of cells, the analysis of the equilibrium state of the potato tissue with an osmotic solution is transposed from the global description of the entire structure down to the analysis of the cell.

Since the vacuole aqueous solution is composed of small amount of minerals and soluble sugars, the solutes constitute the major contribution to the osmotic potential. From the composition of the potato tuber in table 3.9, it can be seen that the main solute constituents are glucose, fructose, sucrose, K_3PO_4, and K_2SO_4. For multicomponent systems, a relationship between the partial water activity of each component and the water activity of the mixture was derived by Ross(1975) considering that all water present in the system forms a solution with each of the components independent of each other:

$$\hat{a}_{wv} = \prod_{j} \hat{a}_{wj} \qquad [3.17]$$

Table 3.8 Water Activity for the Osmotic Solutions.

Solution (%)	FPD (K)	T (K)	$\hat{a}_{wos}^{To}$	m_s (kgs/1000kgw)	$\hat{a}_{wos}^{40}$
5	0.291	272.91	0.9972	0.154	0.9972
10	0.625	272.58	0.9940	0.324	0.9942
20	1.465	271.74	0.9859	0.731	0.9867
30	2.644	270.56	0.9747	1.252	0.9770
40	4.452	268.75	0.9577	1.948	0.9634
60	NA	NA	NA	4.382	0.8956

Table 3.9 Selection of the Representative Composition of the Dry Matter of the Russet Burbank Potato Tubers.

Constituent	Composition (kg/kg dm)
Starch	68.0
Proteins	11.0
Glucose	2.0
Fructose	2.0
Sucrose	1.5
K_2SO_4	1.5
K_3PO_4	4.0
Cellulose	3.0
Others	7.0

modified from Crapiste and Rotstein(1982)

On the basis of equivalent water-j component:

$$\hat{a}_{wj} = 10^{-A_j(1 - x_{wj})^{q_j}} x_{wj} \qquad [3.18]$$

The values of the constants A, q in the eq.[3.18] for various solutes were taken from Crapiste and Rotstein(1982) and are given in table 3.10. The water mole fraction of the j-th component:

$$x_{wj} = \frac{X_v}{X_v + w_j \alpha_j} \qquad [3.19]$$

where:

$$\alpha_j = \frac{M_w}{M_j} \qquad [3.20]$$

At the cytoplasm phase the effects of the numerous interfaces and colloidal materials are important. Thus the prevailing term is the matric potential. Both starch and proteins are important constituents of the cytoplasm. Data for starch in equilibrium with moist air are available in the literature (Nara, 1979). They were correlated by Crapiste and Rotstein(1982):

$$\mu_w - \mu_w^o = \mathbb{R}T \ln \Psi = \mathbb{R}T \ln (1 - \exp(-53.4759X_{st}^{2.3015})) \qquad [3.21]$$

A similar correlation was also developed for proteins in equilibrium with moist air by Crapiste and Rotstein(1982) based on the

Table 3.10 Values of the Constant A and q for various solutes.

Table 3.10 has been removed due to the unavailability of copyright permission.

experimental sorption equilibrium data of Bull(1944) and Hermansson(1977):

$$\mu_w - \mu_w^o = \mathbb{R}T \ln \Psi = \mathbb{R}T\,(-0.0208X_{pr}^{-1.6129}) \qquad [3.22]$$

The total moisture content (X) is calculated from:

$$X = X_v + X_{st}w_{st} + X_{pr}w_{pr} \qquad [3.23]$$

Please note that the contribution of the cell wall phase was considered negligible which is in accordance with the findings of Crapiste and Rotstein (1982).

The last term to be considered is the pressure potential term of the cell. Although Rotstein and Cornish(1978b) found that for the prediction of sorptional equilibrium relationship for apples the pressure potential of the cell (vacuolar phase) could be neglected in the high moisture content region, according to Dainty(1976) the contribution of the pressure potential term, in water relations of plant cells is considered very important under normal growing conditions.

Rotstein and Cornish(1978b) defined the high moisture content region of a sorption isotherm as extending from full turgor down to the moisture content at which the pressure inside the cell (mostly from the vacuole and more generally the cellular volume (V_c) which comprises the cytoplasm and the vacuole in the case of the potato) is equal to the external pressure. This state is named zero turgor or incipient plasmolysis of the cell. The importance of the pressure potential of the plant cell was investigated in the context of an osmotic treatment.

3.3.1.3.1 Full Turgor of the Potato Cell and Potato Tissue

The first case considered was the full turgor state of the cell and tissue. According to Dainty(1976), for small changes in cell volumes, one can write:

$$dP = \xi \frac{dV}{V} \qquad [3.24]$$

Nilsson et al.(1958) have found that the elastic modulus, ξ, is a function of the turgor pressure for potatoes:

$$\xi = \beta_1 P + \beta_2 \qquad [3.25]$$

P is the pressure in excess to the atmospheric pressure.

$$dP = \xi \frac{dV}{V} = (\beta_1 P + \beta_2) \frac{dV}{V} \qquad [3.26]$$

By rearranging the variables, one obtains:

$$\frac{dP}{\beta_1 P + \beta_2} = \frac{dV}{V} \qquad [3.27]$$

Finally the integration is performed to give:

$$P = \left[\left[\frac{V}{V^o} \right]^{\beta_1} \left[P^o + \frac{\beta_2}{\beta_1} \right] \right] - \frac{\beta_2}{\beta_1} \qquad [3.28]$$

Please note that the integration is performed with zero turgor as the reference state in order to compare with literature values in plant physiology. P and P^o are defined as the pressure in excess of the atmospheric pressure. In order to calculate the pressure at full turgor the ratio of the volume at full turgor over the volume at incipient plasmolysis or isotonicity of the cell is needed (V/V^o).

Assuming that the behavior of the biological structure (i. e., the potato tissue) reflects the behavior of the sub units (i. e., the potato plant cell), it is well known from the literature (Noggle and Fritz, 1976) that the volume of the plant cell undergoes a sharp decrease from full turgor to incipient plasmolysis and remains constant for a wide range of concentration of osmotic solutions. Fig. 3.9 shows that experimentally, in the equilibrium study of the potato tissue upon osmosis, the total volume ratio (V/V^o) decreases from full turgor until it reaches a plateau for a wide range of concentration and continues to decrease for highly concentrated sucrose solutions. From a cell point of view, the point of inflection is known as the point at which incipient plasmolysis or isotonicity occurs (Noggle and Fritz, 1976) which in this particular case seems to occur at around 10% osmotic treatment. The ratio between the total volume at full turgor and incipient plasmolysis of the cell is easily determined from the experimental data of the tissue. Table 3.7 shows that $V/V^o = 0.65$ which is the ratio of total volume with respect to full turgor as a reference state. Since incipient plasmolysis has been chosen as a reference state, V/V^o is equal to 1.54. Fig. 3.10 represents the findings of Stadelman(1966) which shows that it is possible for cells with highly

Fig. 3.10 has been removed due to the unavailability of copyright permission.

Fig. 3.10 Diagrammatic Presentation of the Relationship of Cell Volume and Osmotic Quantities in a Cell between Full Turgidity and Turgor Pressure 0 showing a Cell with Highly Stretchable Walls. Abscissa: Relative Cell Volume, V_z, (Volume of the Cell at the State of Incipient Plasmolysis, V_g, is taken as Unity). Ordinate: Suction Potential, S, and Wall Pressure, P, in Relative Values (Suction Potential of the Cell Content at the State of Incipient Plasmolysis, Si_g, is taken as Unity) Stadelman(1966).

N. B. $Si = - RT \ln \hat{a}_{wi}$

$W = \overline{V}_w \Delta P$

$Sz = - RT \ln \hat{a}_{wo}$

stretchable walls to exhibit the same volume ratio. Finally, experimentally Nilsson et al.(1958) have shown that $\beta_1 = 3.5$ and $\beta_2 = 0.5 \times 10^6$ Pa. From eq.[3.28], the pressure at full turgor in excess of the atmospheric pressure can be calculated. It is equal to 5.05×10^5 Pa. Other values of P are calculated for different ratio of volumes. They are reported in table 3.11.

The calculation of ξ and the comparison with literature values was made: for $P = 5.05 \times 10^5$ Pa, $\xi = 22.68 \times 10^5$ Pa; $P = 2.03 \times 10^5$ Pa, $\xi = 12.09 \times 10^5$ Pa. Small values of ξ at low turgor pressure and high values at high turgor pressure were determined. Although no value is published for cells of potato tubers, table 3.12 reports some values for leaves of different higher plant cells. The same trend is observed.

For an hydrostatic pressure in excess of atmospheric pressure of 5.05×10^5 Pa at full turgor, the corresponding water activity inside the cell was calculated ($\hat{a}_{wi}$).

The general equation for chemical potential of water of a potato cell in equilibrium with a solution is written:

$$\mathbb{R}T \ln \hat{a}_{wos} = \mathbb{R}T \ln \hat{a}_{wi} + \bar{V}_w \Delta P \qquad [3.29]$$

where $\hat{a}_{wos}$ is the water activity of the osmotic solution and $\hat{a}_{wi}$ is the water activity inside the cell without the pressure term.

In equilibrium with pure water the potato cell is at full turgor i. e., $\mathbb{R}T \ln \hat{a}_{wos} = 0$:

Table 3.11 Turgor Pressure in Excess of the Atmospheric Pressure as a Function of the Volume Ratio of the Potato Tissue.

V/V_o	$P - P^o$ (Pa)
1.54	5.05×10^5
1.30	2.15×10^5
1.20	1.28×10^5
1.10	0.57×10^5
1.00	0

Table 3.12 Values of ξ Derived from Measurements of the Osmotic Potential as a Function of Water Content of Leaves, by Psychrometry (Dainty, 1976).

Table 3.12 has been removed due to the unavailability of copyright permission.

$$\hat{a}_{wi} = \exp\left[-\frac{\bar{V}_w\,\Delta P}{\mathbb{R}T}\right] \qquad [3.30]$$

$\hat{a}_{wi}$ is found to be 0.9965 at 40°C. From the typical composition reported in table 3.9, given $\hat{a}_{wi} = 0.9965$ and assuming that the $\hat{a}_{wi}$ is the same intantaneously in the cytoplasm and the vacuole, the moisture content of the different phases and the total moisture content can be calculated from eq.[3.18], [3.19], [3.20], [3.21], [3.22], [3.23] where in these equations $\Psi = \hat{a}_{wi}$ and the composition given in table 3.9. The program m.sorp listed in appendix 9 was used to obtain the composition of $X = 5.4578$kg water/kg dry matter; $X_{st} = 0.3769$kg water/kg dry starch; $X_{pr} = 3.0238$kg water/kg dry proteins; $X_v = 4.8689$kg water/kg dry matter at full turgor. A comparison of the calculated results with the experimental value of total moisture content (X) of the full turgor potato material was made. From table 3.5 the total solids measurement of the potato material at full turgor is 15%. The resulting total moisture content on dry matter basis can be calculated, knowing the total solids (TS):

$$X = \frac{(1 - TS)}{TS} \qquad [3.31]$$

Experimentally at full turgor $X = 5.67$kg water/kg dry matter which is very close to the calculated value. From this, on can assume that the composition listed in table 3.9 represents the composition of the potato selected from the experimental work. It also illustrates the fact that the pressure term is important.

3.3.1.3.2 Case of Stored Potato Material

The second case under investigation was the state of the stored potatoes. In the literature the cell sap measurement by freezing point depression is a direct determination of the osmotic potential of the fresh tissue. The values from Salisbury and Ross(1969) are reported in table 3.13. The highest value of cell sap measurement or osmotic potential was found to be 8.51×10^5 Pa and the lowest 2.23×10^5 Pa. However, the osmotic potential really depends on the state of the fresh or stored potato from which measurements were made. Noggle and Fritz(1976) pointed out that, under normal growing conditions, the state of the potato tissue varies reversibly between full turgor and incipient plasmolysis depending on the conditions of the environment. The fresh material is known to be turgid. Experimentally the total water content (X) of the stored material was found to be 4.00kg water/kg dry matter. The calculation of the water activity was done in order to match the experimental value of total moiture content (X) using eq.[3.18], [3.19], [3.20], [3.21], [3.22], [3.23] and the composition in table 3.9, using the program m.sorp. A comparison was made with the literature value for fresh tissue. Given a $X = 4.0712$kg water/kg dry matter; $X_{st} = 0.3675$kg water/kg dry starch; $X_{pr} = 2.4765$kg water/kg dry proteins; $X_v = 3.5487$kg water/kg dry matter, one obtains the corresponding $\hat{a}_{wi} = 0.9952$. The cell sap values reported in the literature are expressed with the unit of pressure (OP):

Table 3.13 Cryoscopically Determined Osmotic Potentials for Plant Extracts Obtained in Several Different Ways (Salisbury and Ross, 1969).

Table 3.13 has been removed due to the unavailability of copyright permission.

$$OP = - \frac{\mathbb{R}T \ln \hat{a}_{wi}}{\bar{V}_w} \qquad [3.32]$$

At 40°C, OP = 6.96×10^5 Pa. This value is within the range of the cell sap values reported by Salisbury and Ross(1969) in table 3.13. No correction was made for the temperature since the effect is negligible in this particular case.

3.3.1.3.3 **Case of Incipient Plasmolysis**

The last case to investigate, concerning the influence of the pressure term, was to define the water activity and the composition of the potato cell or tissue at which incipient plasmolysis is reached (i. e., the pressure potential term is not present anymore). Fig. 3.9 seems to indicate that the potato tissue plasmolyzes at solution concentration between 5% to 10% sucrose. A constant total volume is reached. The water content of the potato material in equilibrium with a 5% osmotic solution (X = 4.13kg water/kg dry matter) is approximately equal to the water content of the fresh material (X = 4.00kg water/kg dry matter). From table 3.8, it can be seen that, in order for the material to plasmolyze, the concentration of the osmotic solution has to be more than 5% which has a $\hat{a}_{wos} = 0.9972$. It was found that for the potato material at full turgor $\hat{a}_{wi} = 0.9966$ and, also, that for the stored potato material $\hat{a}_{wi} = 0.9952$. Because of the increase in cell sap concentration due to the loss of water and consequently the decrease in cell size or volume from full turgor to incipient plasmolysis, the osmotic potential ($\mathbb{R}T \ln \hat{a}_{wi}$) is expected to increase from full turgor to incipient plasmolysis. Furthermore, the $\hat{a}_{wi}$ should decrease as the concentration of solutes become important. At incipient plasmolysis, the pressure potential term is zero so that:

$$\mathbb{R}T \ln \hat{a}_{wos} = \mathbb{R}T \ln \hat{a}_{wi} \qquad [3.33]$$

Table 3.8 lists the water activity of the osmotic solution as calculated by eq.[3.15] and corrected for the temperature using eq.[3.16]. The experimental total water content of the potatoes (X) on a dry matter basis for each concentration of sucrose solution was calculated by eq.[3.31]. There is a measurable uptake of sucrose by the potato material assumed to be in the extracellular volume so that:

$$X = X_i \frac{\Delta SC}{TS} + X_c \frac{TS - \Delta SC - W}{TS} \qquad [3.34]$$

where X is obtained experimentally and defined as the water content of the osmosed potato on a dry matter basis, X_i is the water of the sugar solution in the extracellular space on a sucrose basis, X_c is the water content of the cellular volume on a dry matter of cellular space basis, ΔSC is the difference between the sugar content of the osmosed potato and the conditioned potato as measured by HPLC, TS is the total solids of the treated potato and finally W is the proportion of the osmosed potato that is considered cellulose or others which is not a part of the cellular volume. Since there is a change in total mass upon osmosis as well as a change in composition especially sucrose, W is defined:

$$W = \frac{\omega_w \, TS^o}{(1 + \frac{ML}{100})} \qquad [3.35]$$

where TS^o is the total solids of the fresh material (20%) and ML the mass loss due to the treatment. The water activity inside the cell is calculated using eq.[3.18], [3.19], [3.20], [3.21], [3.22], [3.23] and the composition in table 3.9 using the program m.sorp in order to match the final moisture content, X_c, obtained by eq.[3.34] and eq.[3.35].

Table 3.14 reports the values of water activity inside the potato cell. Fig. 3.11 represents the results of the water activity inside and outside the potato cell which was in equilibrium with an osmotic solution at 40°C. They are reported as a function of the sucrose concentration of the osmotic solution. The point at which the curve of $\hat{a}_{wos}$ intersects the curve $\hat{a}_{wi}$ is the value of water activity corresponding to incipient plasmolysis and the sucrose concentration of the osmotic solution seems to be around 20% although from the experimental volume, the sucrose concentration of the osmotic solution at incipient plasmolysis appears to occur at around 10%. According to Garcia and McFelley(1978) and Lenart and Flink(1984a) the isotonicity occurs in a 10% sucrose solution. However, the value being reported as isotonic is in fact the value where the fresh tissue shows no change in volume after treatment in this particular sucrose solution (Salisbury and Ross, 1969). Furthermore, Willis and Teixera(1988) have also found a great variability in experimental results around plasmolysis.

Table 3.14 Calculation of the Water Activity inside the Cellular Volume of the Potato Tissue in Equilibrium with an Osmotic Solution at 40°C from the Experimental Measurements of Total Solids (TS), Sugar Content (SC) and mass loss (ML).

Solution (%)	X (kg/kg)	$X_i \frac{\Delta SC}{TS}$ (kg/kg)	$X_c \frac{TS-\Delta SC-W}{TS}$ (kg/kg)	X_c (kg/kg)	$\hat{a}_{wi}$
5	4.13	0	4.13	4.13	0.9953
10	2.85	1.51	1.34	1.86	0.9885
20	2.13	1.21	0.92	1.52	0.9855
30	1.53	0.98	0.55	1.08	0.9779
40	1.18	0.76	0.42	0.97	0.9747
60	0.53	0.34	0.19	0.44	0.9228

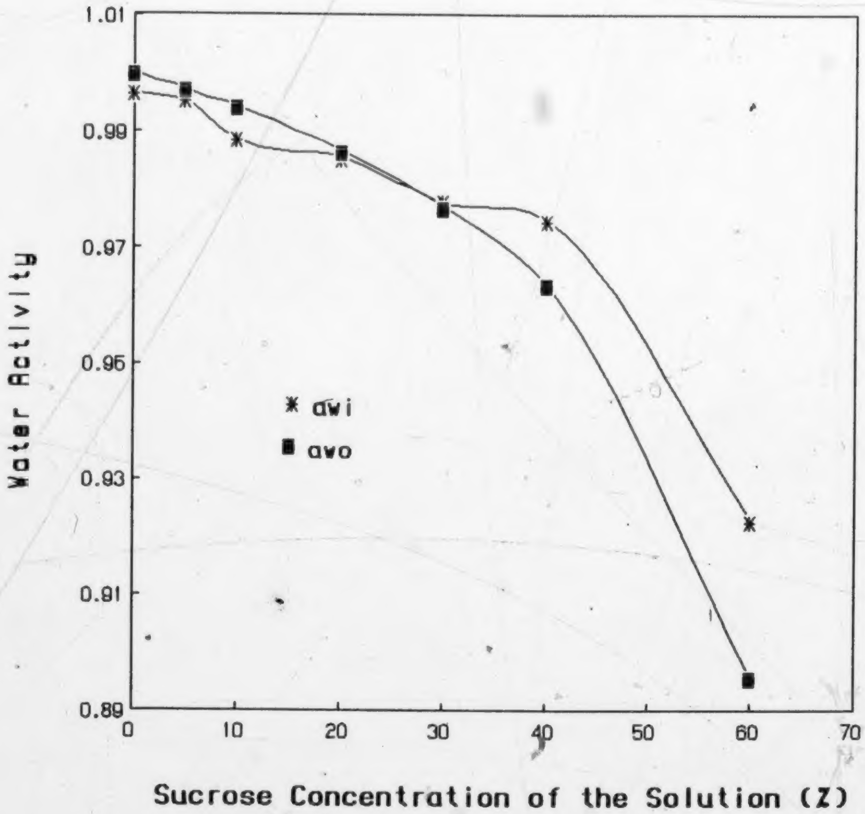

Fig 3.11. Concentration of Sucrose Solution at Incipient Plasmolysis

The values of Ψ were also estimated by different correlations from the literature in order to compare. A correlation developed by Ratti et al.(1988):

$$\ln \Psi^{R} = Q(X)\ \ln P + C(X) \qquad [3.36]$$

where P is the vapor pressure of water at 313K. It is equal to 7.375 kPa and:

$$Q(X) = q_1\ \exp(-q_2X)\ X^{q_3} \qquad [3.37]$$

$$C(X) = c_1\ \exp(-c_2X)\ X^{c_3} \qquad [3.38]$$

For potatoes: $c_1 = -2.67 \times 10^{-2}$; $c_2 = 0$; $c_3 = -1.656$;
$q_1 = 0.0107$; $q_2 = 1.287$; $q_3 = -1.513$.

The Hasley(1948) correlation which provides a good fit for the high moisture content region was used also to calculate Ψ^{H} knowing the experimental moisture content (X):

$$\Psi^{H} = \exp\left[\frac{-B}{\mathbb{R}T}\ \frac{1}{X^{c}}\right] \qquad [3.39]$$

where: $B = 5.586 \times 10^{4}$; $c = 1.648$; $T = 313K$. Table 3.15 shows the comparison between the calculated values of $\hat{a}_{wi}$ and $\hat{a}_{wos}$ and the correlated values, Ψ^{R} and Ψ^{H}. Both correlations provide an acceptable fit.

Finally, it can be seen that osmotic drying processes operate in the high moisture content region. Table 3.15 shows that, empirically, the correlations provide an acceptable fit. However, the pressure potential term should be included particularly in further modelling.

3.3.1.4 Comparison Between the Experimental Equilibrium Parameters of the Potato Tissue and the Corresponding Calculated Equilibrium Parameters Involving the Different Phases of the Potato Cell

The calculations of the water loss or mass loss as well as the contribution of the different phases such as the vacuole and the cytoplasm with respect to water or mass loss were done based on the sub units behavior neglecting the pressure potential term and compared with the experimental results of water and mass loss and sugar gain of the potato tissue. The mass of dry matter was assumed to remain constant.

Table 3.8 reports the values of $\hat{a}_{wos}$ for different osmotic solutions. The value of moisture content (X^o) at full turgor is available experimentally as being 5.67kg water/kg dry matter which corresponds to a Ψ of 0.9985 or 0.9987 from the Ratti et al.(1988) and Hasley(1948) correlations. Assuming that the potato tissue is in equilibrium with an osmotic solution of known $\hat{a}_{wos}$, the total moisture content (X) of can be calculated from either the Ratti or Hasley correlation, the water loss by the potato cell (WL^{cal}) is defined by:

$$WL^{cal} = \left[\frac{X}{X^o} - 1 \right] \omega_w \qquad [3.40]$$

Table 3.15 Comparison between the Water Activity of the Potato Tissue ($\hat{a}_{wi}$) in Equilibrium with an Osmotic Solution ($\hat{a}_{wos}$) at 40°C with the Water Activity Calculated from Empirical Correlations.

Solution (%)	$\hat{a}_{wi}$	$\hat{a}_{wos}$	Ψ^R Ratti et al.	Ψ^H Hasley
Full Turgor	0.9966	1.0000	0.9985	0.9987
5	0.9953	0.9972	0.9975	0.9979
10	0.9886	0.9942	0.9913	0.9924
20	0.9855	0.9867	0.9884	0.9894
30	0.9779	0.9770	0.9815	0.9814
40	0.9747	0.9634	0.9786	0.9778
60	0.9228	0.8956	0.9401	0.9205

where X is the total moisture content of the osmosed potato material, X^o is the total moisture content of the full turgor material and ω_w is the proportion of water in the full turgor potato material.

Eq.[3.21] and eq.[3.22] are used to calculate the moisture content of the starch (X_{st}) and proteins (X_{pr}). The water loss by the cytoplasm (WL_{cy}^{cal}) is determined by:

$$WL_{cy}^{cal} = \left[\frac{X_{st}^o \, w_{st}}{X^o} \left[\frac{X_{st}}{X_{st}^o} - 1 \right] + \frac{X_{pr} \, w_{pr}}{X^o} \left[\frac{X_{pr}}{X_{pr}^o} - 1 \right] \right] \omega_w \qquad [3.41]$$

Eq.[3.23] is used to calculate by difference the moisture content of the vacuole, X_v. The water loss of the vacuole is:

$$WL_v^{cal} = \left[\frac{X_v^o}{X^o} \left[\frac{X_v}{X_v^o} - 1 \right] \right] \omega_w \qquad [3.42]$$

This hypothetical system represents the potato cells in contact with a medium which influences the loss of water of these structures which, in this case, also equals the mass loss.

The values of total moisture content (X), the water content of the starch (X_{st}) and proteins (X_{pr}) are reported in table 3.16 together with the concentration of the sucrose solution.

On fig. 3.12, the calculated total water loss (WL^{cal}), the water loss by the cytoplasm (WL_{cy}^{cal}) and the vacuole (WL_v^{cal}) are plotted against the sucrose concentration of the osmotic solution with the

Table 3.16 Values of Total Moisture Content (X), Water Content of the Starch (X_{st}) and Proteins (X_{pr}) and Moisture Content of the Vacuole (X_v) of the Potato cell in Equilibrium with an Osmotic Solution at 40°C.

Sucrose Solution (%)	X (kg/kg)	X_{st} (kg/kg)	X_{pr} (kg/kg)	X_v (kg/kg)
0	5.6667	0.4021	5.3261	4.8074
5	3.4387	0.3831	3.4641	2.7971
10	2.2084	0.3617	2.2034	1.7201
20	1.3316	0.3351	1.3140	0.9592
30	0.9522	0.3160	0.9328	0.6347
40	0.7153	0.2984	0.6964	0.4358
60	0.3705	0.2529	0.3555	0.1594

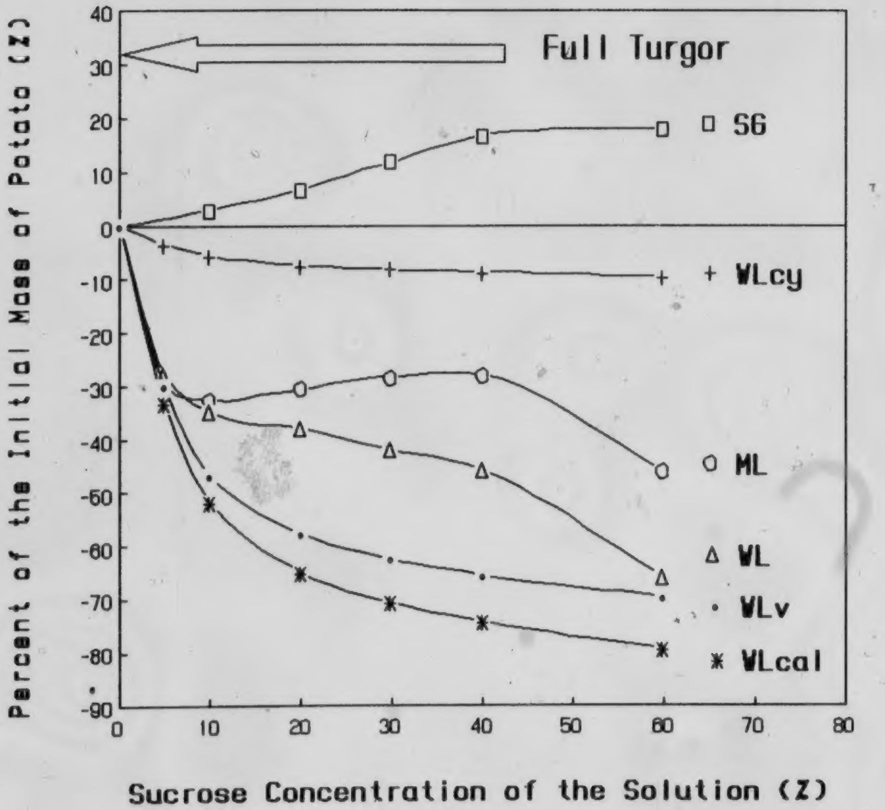

Fig. 3.12. Experimental and Calculated Equilibrium Parameters.

experimental results of mass loss (ML), water loss (WL) and sugar gain (SG). Table 3.17 reports also the same results.

From full turgor to a 10% sucrose solution, the experimental water loss and weight loss are similar to the calculated ones. The contribution of the vacuole is the most important one as compared to the contribution of the cytoplasm. It can be expected that the main contribution will come from the vacuole because the water activity of all osmotic solutions is fairly high.

From a 10% to a 60% osmotic solution, the uptake of sugar is so important that the discrepancy between the calculated and experimental water and weight loss becomes significant. However, not only sucrose is gained by the biological structure, sucrose and water as a solution enters the potato material. Consequently, the experimental water and mass loss is less than the calculated ones.

It has to be pointed out that the water content of the potato material at full turgor is higher than the water content of the potato material at full turgor reported by Crapiste and Rotstein (1982) and other workers in the field of sorptional equilibrium data. This was probably due to the conditioning step that was performed experimentally.

The changes occurring in the different phases of the potato cell were investigated and compared with the experimental changes occurring in the potato tissue. Some discrepancies were found particularly related to the increase of the sugar uptake by the structure. In order to fully understand and explain the phenomenon, the behavior of the different phases of the cell were considered in terms of volumes and compared with the experimental volumes.

Table 3.17 Calculated Equilibrium Parameters of Total Water Loss (WL^{cal}), Water Loss by the Cytoplasm (WL_{cy}^{cal}) and Water Loss by the Vacuole (WL_{v}^{cal}) of the Potato Cell in Equilibrium with an Osmotic Solution at 40°C.

Sucrose Solution (%)	WL^{cal} (%)	WL_{cy}^{cal} (%)	WL_{v}^{cal} (%)
5	-33.42	-3.27	-30.15
10	-51.87	-5.56	-46.31
20	-65.03	-7.30	-57.72
30	-70.72	-8.13	-62.59
40	-74.27	-8.70	-65.57
60	-79.44	-9.72	-69.72

3.3.1.5 Comparison Between the Experimental Volumes of the Potato Tissue and the Corresponding Equilibrium Calculated Volumes of the Different Phases Present in a Potato Cell

Assuming that the mass of dry matter (m_{dm}) remains constant, the calculated cell volumes were determined on a dry matter basis:

$$\frac{V}{m_{dm}} = \frac{X}{\rho_w^*} + \frac{1}{\rho_{dm}^*} \qquad [3.43]$$

The volume of the cytoplasm is calculated in the following manner.

$$\frac{V_{cy}}{m_{dm}} = \left[\frac{X_{st} w_{st}}{\rho_w^*} + \frac{w_{st}}{\rho_{st}^*} \right] + \left[\frac{X_{pr} w_p}{\rho_w^*} + \frac{w_{pr}}{\rho_{pr}^*} \right] \qquad [3.44]$$

Finally, the volume of the vacuole is estimated by difference.

$$\frac{V_v}{m_{dm}} = \frac{V}{m_{dm}} - \frac{V_{cy}}{m_{dm}} \qquad [3.45]$$

On fig. 3.13, the volumes are reported as a proportion of the initial total volume and plotted against the sucrose concentration of the osmotic solution with the cellular volume obtained from the experimental data. Fig. 3.13 and table 3.18 show that from full turgor to incipient plasmolysis the vacuole undergoes the major decrease in volume. In a 20% sucrose solution, the volume of the vacuole becomes smaller than the volume of the cytoplasm. Fig. 3.13 shows also that the

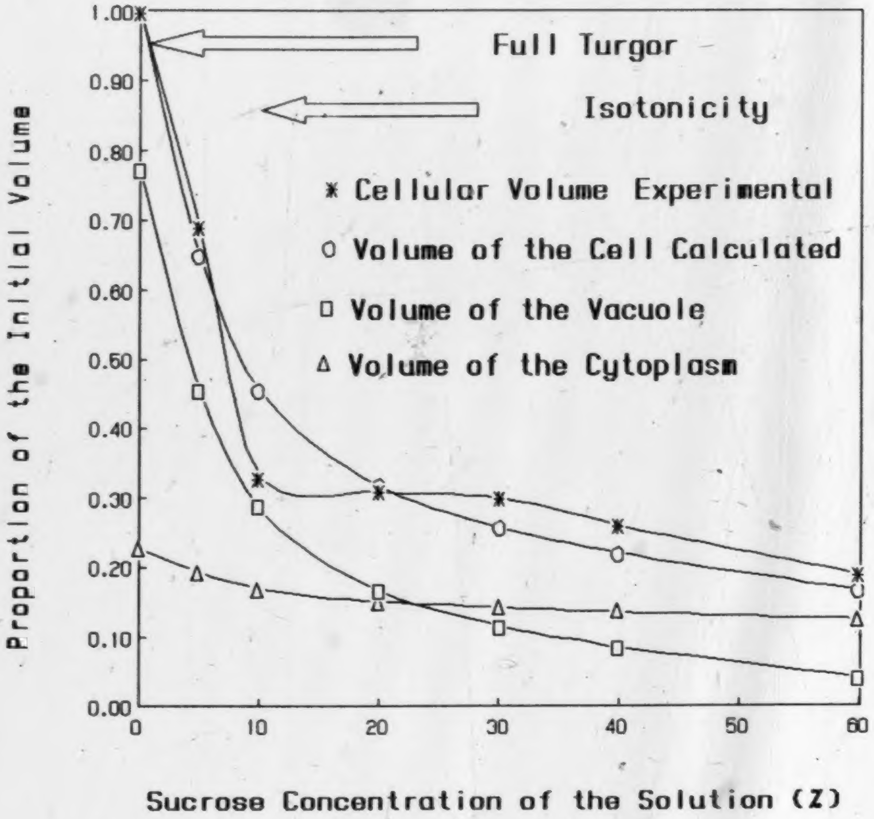

Fig. 3.13. Experimental and Calculated Volume Changes.

Table 3.18 Calculated Parameters: Cellular Volume (V_c/V^o), Volume of the Vacuole (V_v/V^o) and Volume of the Cytoplasm (V_{cy}/V^o) of the lumped Potato Cells in Equilibrium with an Osmotic Solution at 40°C Reported as a proportion of the initial Volume.

Sucrose Solution (%)	Cellular Volume V_c/V_o	Volume of the Vacuole V_v/V_o	Volume of the Cytoplasm V_{cy}/V_o
Blank	1.0	0.7728	0.2272
5	0.6493	0.4564	0.1930
10	0.4558	0.2869	0.1689
20	0.3178	0.1672	0.1506
30	0.2581	0.1161	0.1420
40	0.2208	0.0848	0.1360
60	0.1666	0.0413	0.1252

experimental cellular volume of the tissue matches the calculated cell volume.

This implies two major consequences: first, sucrose is a true impermeable, which means that it does not enter the cellular volume of the tissue, second, in such a system the water loss by the cellular volume of the tissue upon osmotic treatment can be accounted from a cell point of view taking into account the contribution of the different phases such as vacuole and cytoplasm present in the cellular volume. Consequently, on can infer the repartition of water and sugar in the cellular volume of the potato material.

However, discrepancies occur because of the behavior of the extracellular space. In an osmotic process, the extracellular volume is filled up with the solution preventing the collapse of the structure. The water loss is slowed down and the sugar is gained by the biological structure. Moreover, Mazza(1983) has found that the texture of osmotically dried material is more or less open and rigid and the tissue does not collapse as much as compared to air dried material.

3.3.1.6 Summary of the General Behavior of a Plant Cell Undergoing an Osmotic Treatment

The summary of the general behavior of a plant cell undergoing an osmotic treatment is described here and shown on the fig. 3.14.

Starting at full turgor, the extracellular space of the cell is minimum. The cellular volume pushes the wall (fig. 3.14 a). As water is lost by the cell coming from the cellular volume, the total volume is affected whereas the extracellular volume stays constant.

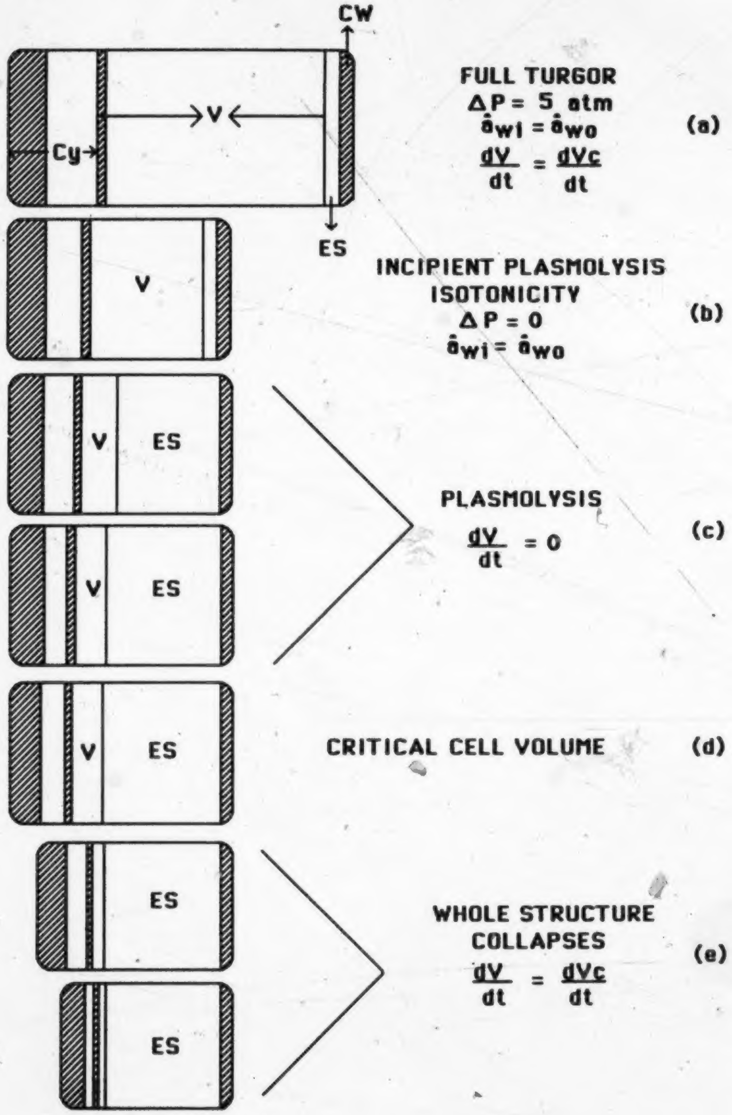
CW
Cy
V
ES
FULL TURGOR
$\Delta P = 5$ atm
$\hat{a}_{wi} = \hat{a}_{wo}$
$\frac{dV}{dt} = \frac{dV_c}{dt}$
(a)
INCIPIENT PLASMOLYSIS
ISOTONICITY
$\Delta P = 0$
$\hat{a}_{wi} = \hat{a}_{wo}$
(b)
PLASMOLYSIS
$\frac{dV}{dt} = 0$
(c)
CRITICAL CELL VOLUME
(d)
WHOLE STRUCTURE
COLLAPSES
$\frac{dV}{dt} = \frac{dV_c}{dt}$
(e)

Fig. 3.14 Physiological Representation of the Shrinkage Behavior.

As soon as incipient plasmolysis or isotonicity (fig. 3.14 b)is reached, any further loss in cellular volume is compensated by a proportional increase in extracellular space (fig. 3.14 c).

Up to this point, this typical shrinkage behavior applies in most conditions of an osmotic treatment (range 10%-40% osmotic solution) at equilibrium. The osmotic treatment of a potato tissue in a 60% sucrose solution appears to involve a different shrinkage behavior. Table 3.8 shows that the total volume is significantly smaller in a 60% osmotic solution. The extracellular space is also smaller than in a 40% sucrose solution as well as the cellular volume. As pointed out by Toupin(1986), a third stage of dehydration is characterized by the fact that the cell membrane starts to pull the cell wall inward, its point of anchorage causing the collapsing of the structure when a critical cell volume (or volume at which the intrinsic properties of the plant cell are lost) is reached (fig. 3.14 d,e). The behavior of the potato tissue in a 60% osmotic solution could be explained by the fact that the cell wall is collapsing. Moreover, in conventional drying process, pratical conditions of dehydration are, to a large extent, governed by the necessity of minimizing the irreversible loss of the elasticity of the cell walls occurring in this last stage of dehydration (Van Arsdel, 1963). However the irreversible loss of elasticity of the cell wall has been found to occur at very low water activity (Willis and Teixeira, 1988). Furthermore, studies on rehydration properties of celery conducted by Willis and Teixeira(1988) reveal that the loss of the membrane integrity is also an important factor which impairs the rehydra.ability of fruits and vegetables. Irreversible loss of rigidity upon rehydration which is controlled by the selective permeability of the membrane was observed as the membrane was chemically destroyed using ethanol. It usually occurs much earlier than the loss of elasticity of the cell wall in the process (Willis and Teixeira, 1988).

3.3.1.7 **Miscellaneous Observations Occurring during the Osmotic Treatment**

Some qualitative observations were recorded along the process. Shrinkage was found to occur in three directions like in conventional drying (Van Arshel, 1963).

During the preliminary experiments establishing the procedure of the equilibrium study some osmosed samples were kept in the cold room at 4°C for two weeks prior to sugar analysis. Sugars were then analyzed by HPLC. A very important enzyme activity was found, the sucrose being degraded into glucose and fructose. From a processing point of view, if sucrose is chosen as a solute, the enzymes probably located in the cell wall must be inactivated as soon as possible after the osmotic treatment.

Foaming and a sour smell was observed when the osmotic treatment was conducted with a 10%-30% sucrose solution. The phenomenon was found to appear late, during the second half of the treatment.

3.3.2 **Kinetic Study**

Problems in the design of an operation such as dehydration, packaging, storage and particularly osmotic concentration arise when a foodstuff is removed from an equilibrium situation and is required to reach a new one. Roman et al.(1983) reported that, in drying, much less attention has been given to the kinetics of the phenomenon by which equilibrium is attained. Moreover, Lenart and Flink(1984b) indicated that, in the area of osmotic concentration, very little has been published regarding the spatial distribution of the water and solute(s) in the biological structure as a function of time. As a general rule, increasing the concentration of solute in the osmotic solution or increasing the time of osmosis gives an increase in osmosis penetration. Since time is the limiting factor most of the authors suggest to operate at high concentration rather than longer time. However, the results of the equilibrium study have shown that an optimum would have to be found between concentration and contact time.

Fig. 3.15, fig. 3.16 and fig. 3.17 report the measurement of density of the potato slices for three time levels (i. e., 1 hour, 6 hour and 24 hour treatment) in a 20%, 40% and 60% sucrose solution as a function of the depth of penetration in the tuber. The density increases from the surface to a depth sufficiently far from the centre particularly for highly concentrated sucrose solution. The steepness of the profile increases as the concentration of the solution increases. The measurements of density have been used to estimate the position of the slice through the mass of the potato sample which is the common determination relating the measurement of moisture content, sugar content and density measurement. The reader is referred to appendix 10 for details on the transformation.

Fig. 3.18, fig. 3.19 and fig. 3.20 represent the measurement of sugar content as a function of the depth of penetration in the slice for three treatments 20%, 40% and 60% sucrose solution and three time durations of treatment (i. e., 1 hour, 6 hour and 24 hours). For a 24 hour treatment, there is saturation of the first layer of approximately

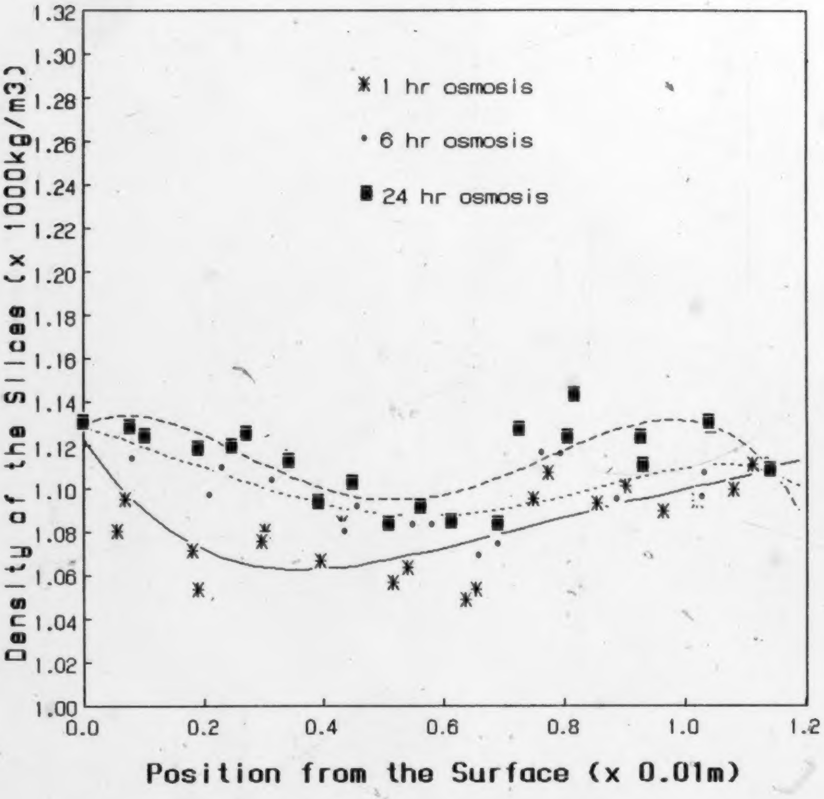

Fig. 3.15 Density versus Position for a Treatment in a 20% Sucrose Solution.

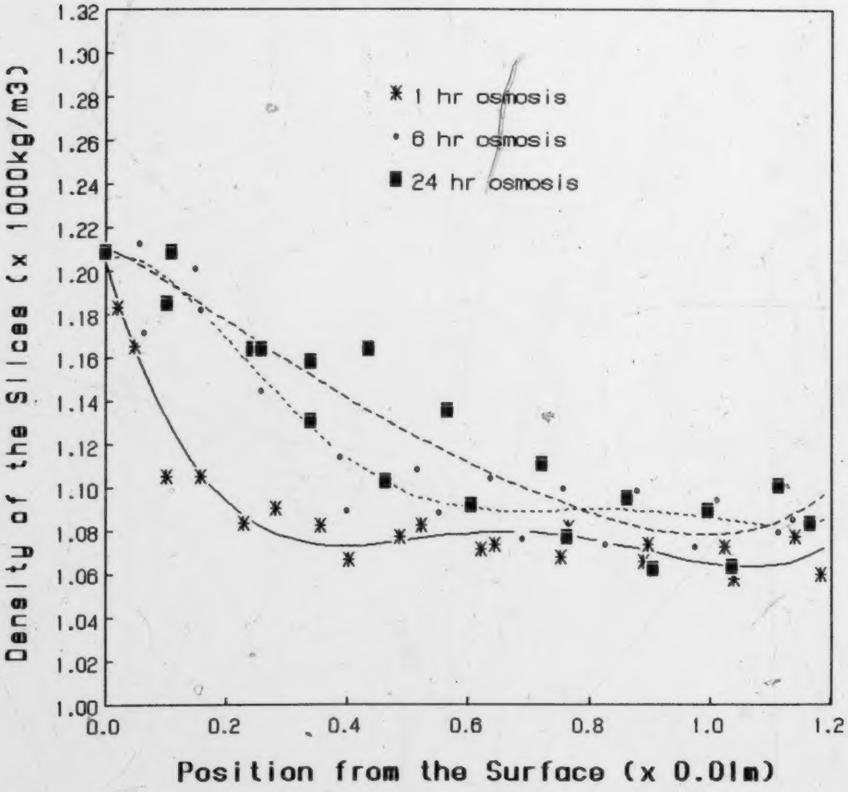

Fig. 3.16 Density versus Position for a Treatment in a 40% Sucrose Solution.

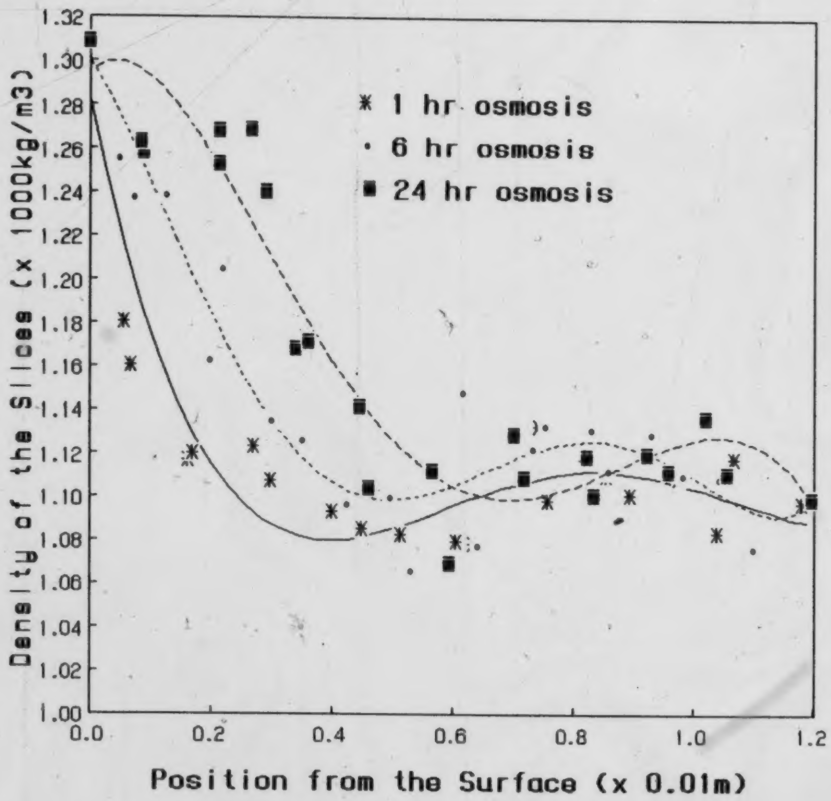

Fig. 3.17 Density versus Position for a Treatment in a 60% Sucrose Solution.

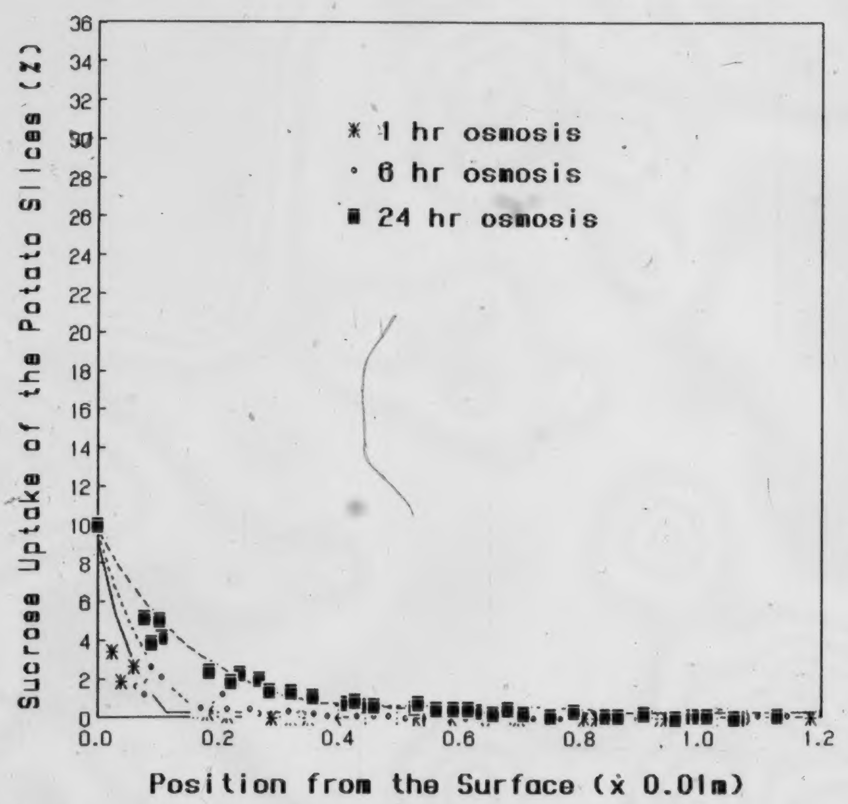

Fig. 3.18 Sucrose Uptake versus Position for a Treatment in a 20% Sucrose Solution.

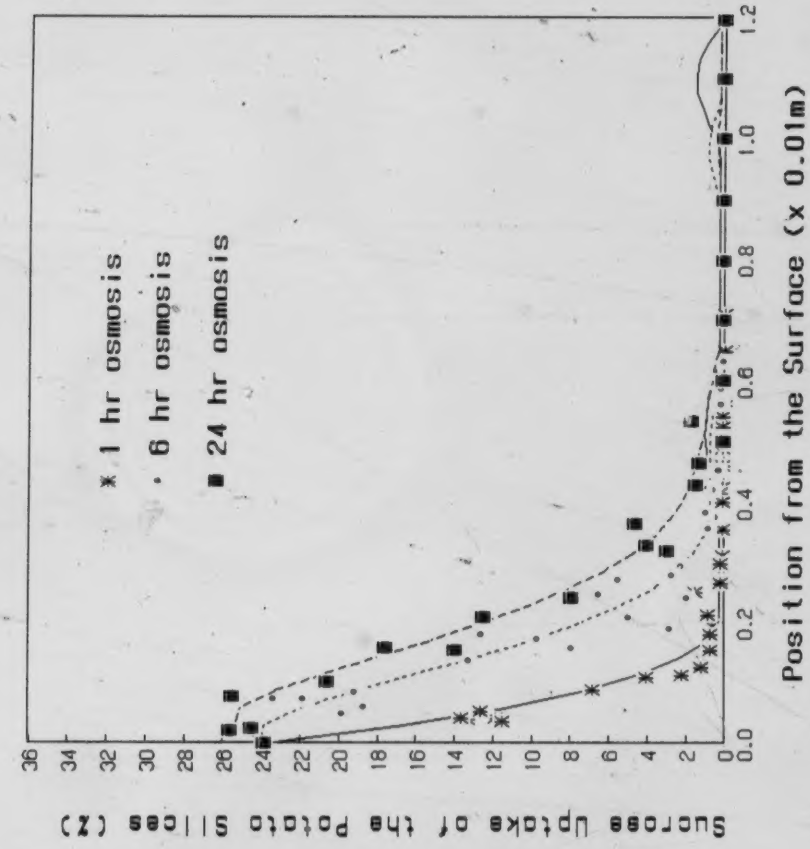

Fig. 3.19 Sucrose Uptake versus Position for a Treatment in a 40% Sucrose Solution.

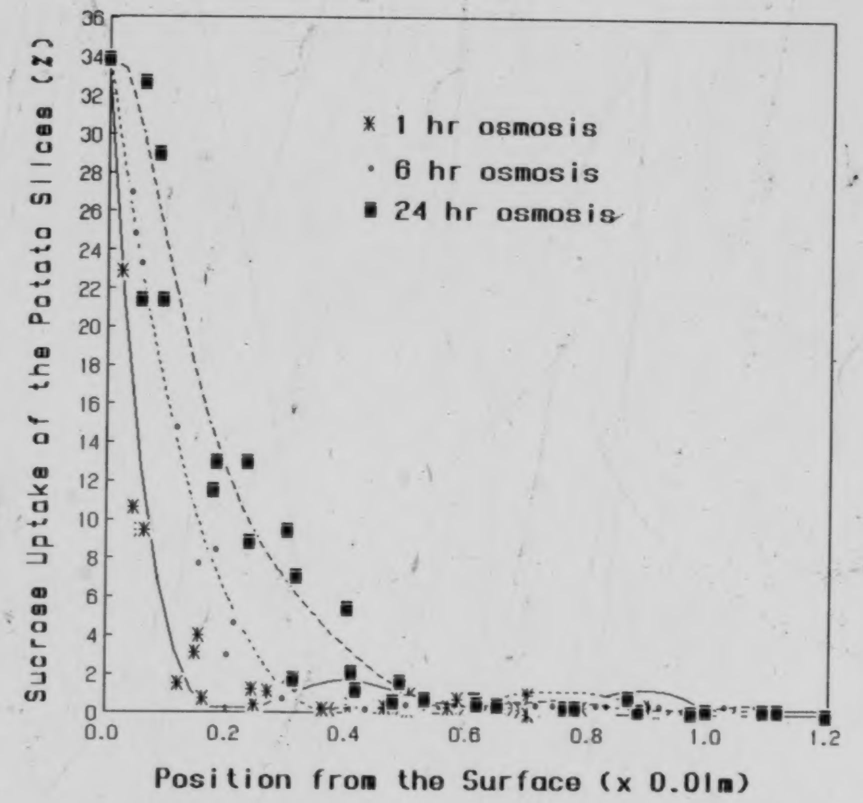

Fig. 3.20 Sucrose Uptake versus Position for a Treatment in a 60% Sucrose Solution.

2×10^{-3} m followed by a sharp decrease. This type of behavior is observed for a treatment in a 40% and 60% sucrose solution whereas the sugar seems to be washed out for a treatment in a 20% osmotic solution. The saturation of the layer of approximately 2×10^{-3} m is also a time function. For a treatment in a 40% sucrose solution, it occurs as early as in 6 hours.

The data on the moisture content measurement for the three time level of treatment and the three concentrations of sucrose solution confirm the observations made for the sucrose content measurements (fig. 3.21, fig. 3.22 and fig. 3.23). In a 20% sucrose solution, the water content measurements reflect the fact that there is little penetration of sugar in the potato material. The values of moisture content for a treatment in a 40% sucrose solution agree with the fact that there is saturation of the first layer particularly for a 6 hour and 24 hour treatment. The same moisture content profile is observed for a 60% sucrose solution. Although, according to the moisture content data, the saturation of the first layer appears to occur earlier (i. e., for 6 hour osmotic treatment) than the data on sucrose content seem to indicate.

Please note that the values at the surface (z=0) correspond to the equilibrium data.

The equilibrium study has shown that the extracellular space increases dramatically when the cell reaches plasmolysis. Since sucrose penetrates in the extracellular space, the mass transport of this species is favored, not only by a difference in chemical potential between the solution side and the potato material but, also, by an

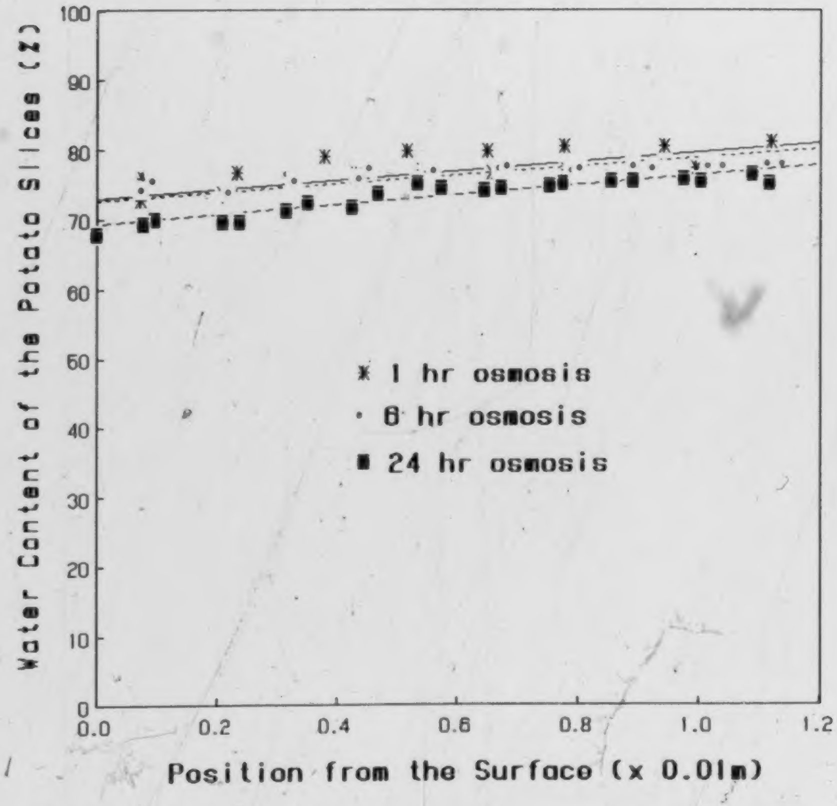

Fig. 3.21 Moisture Content versus Position for a Treatment in a 20% Sucrose Solution.

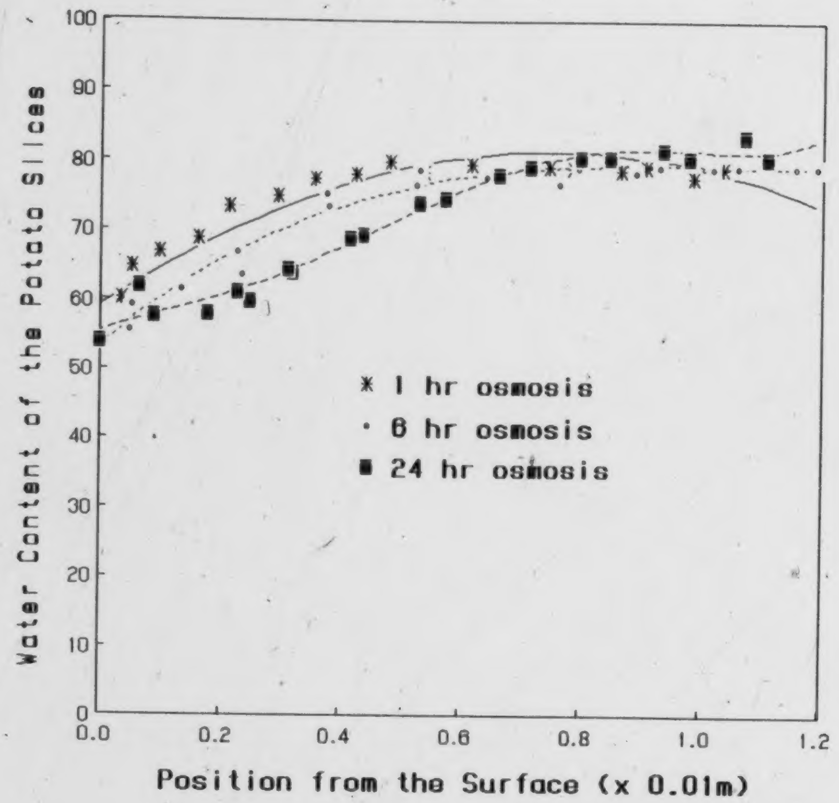

Fig. 3.22 Moisture Content versus Position for a Treatment in a 40% Sucrose Solution.

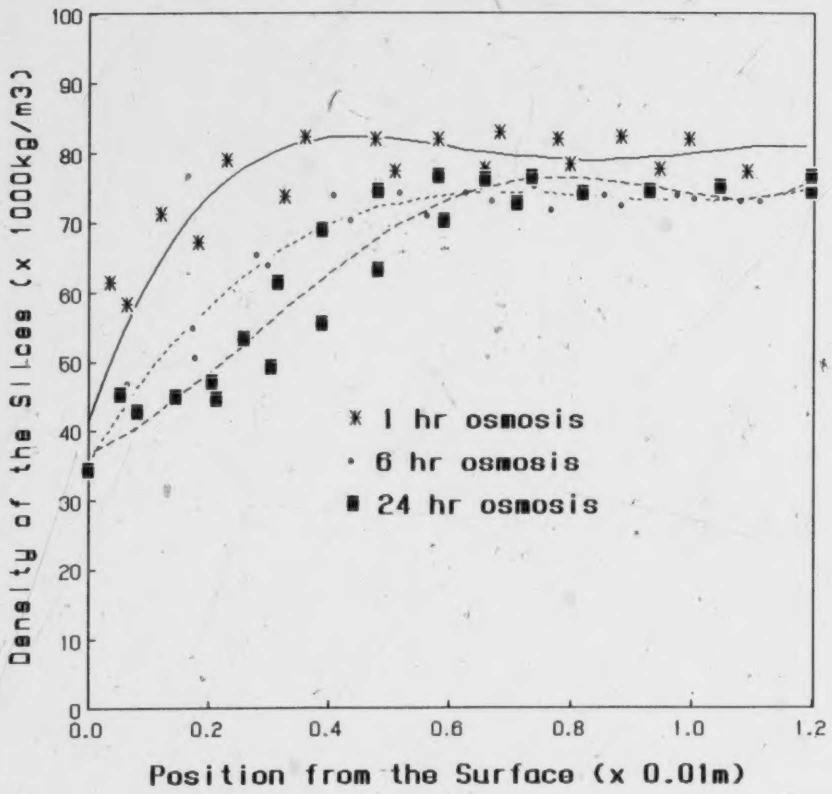

Fig. 3.23 Moisture Content versus Position for a Treatment in a 60% Sucrose Solution.

increase in the surface area of extracellular space which has an effect on the penetration of sucrose.

From the equilibrium study, it was also found that a solution of at least 10% to 20% would allow for plasmolysis to occur (table 3.7 and fig. 3.11). In these conditions the surface cells of the potato exposed to a 20% osmotic solution are expected to be on the border line of plasmolysis. The extracellular space of these cells is therefore limited to the initial value at full turgor if they are not plasmolysed (i. e., approximately 4.0% of the initial total volume). For treatments in a 40% or 60% sucrose solution, the surface cells are most likely to be plasmolysed which corresponds to a proportion of extracellular volume, with respect to the total volume at full turgor of 38%. Furthermore the extracellular space has increased by 709% since the volume of extracellular space has increased from 4.0% to 38% (table 3.7). The sugar can more easily penetrate. This and also the fact that the difference in chemical potential on both sides is more important than for a treatment in a 20% osmotic solution contribute to the experimental differences in mass transport of sugar inside the structure. In summary, the combined effect of difference in chemical potential between the solution and the potato material and the mass transfer surface area increase affect the transport properties of sucrose and water inside the structure.

Finally, the kinetic study shows that the penetration of sugar is slow. Shrinkage pattern affects the transport properties of sugar and water inside the structure. The surface available for transport (i. e., the extracellular volume) increases as sugar penetrates the potato structure. As the surface area of transport increases, the flux of sugar is considerably reduced because of the expansion effect. The penetration of sugar is slowed down. These considerations will be used in further modelling.

4. MODELLING OF THE OSMOTIC TREATMENT OF POTATO TISSUE IN A SUCROSE SOLUTION

4.1 Mathematical Representation of the Tissue

The modelling of the mass transfer of water and sucrose in potato tissue upon osmosis requires the definition of a realistic simplified representation of a biological structure in terms of physical dimensions and shape. Because of the relative coherence that exists in plant storage tissue (e. g., potato tissue), one can define a unit cell, as a representative microscopic unit of the structure, characterized by the average typical properties of the real cells. Fig. 4.1a shows a simplified representation of an average unit cell of potato parenchyma tissue. Fig. 4.1b represents a cubic arrangement of these average unit cells in a tissue structure. The analysis of mass transport of the entire structure upon osmosis is transposed from the global description down to the analysis of the behavior of the average unit cell in this particular arrangement (Toupin, 1986). The anisotropy of such structure introduces some major difficulties in describing the apoplast transport or diffusive flow in the extracellular space.

Toupin(1986) developed the concept of the equivalent cylindrical unit cell (ECUC) and proposed an arrangement of these ECUC in an hypothetical parenchyma tissue in order to avoid this particular constraint. Fig 4.2a shows the ECUC. Each cell is represented as three coaxial cylinders. The cylinder no:1 acts as a buffer. The cylinder no:2 represents the extracellular volume which includes the cell wall and the free space. The cylinder no:3 comprises the cellular volume with its vacuole and cytoplasm. Fig 4.2b shows that the hypothetical

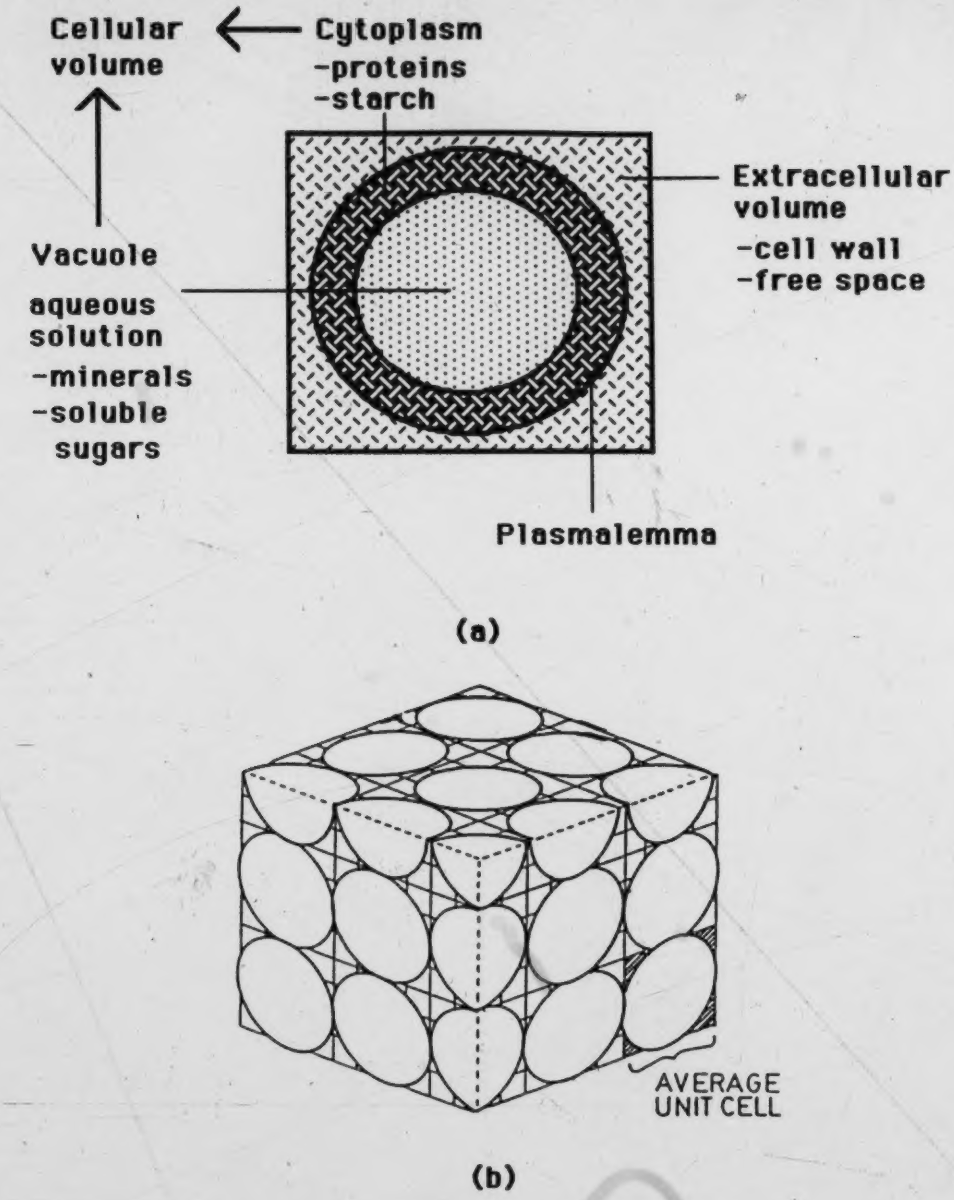
Cellular volume
Cytoplasm
-proteins
-starch
Extracellular volume
-cell wall
-free space
Vacuole
aqueous solution
-minerals
-soluble sugars
Plasmalemma
(a)
AVERAGE UNIT CELL
(b)

Fig. 4.1 (a) Average Unit Cell (b) Cubic Arrangement of Average Unit Cells.

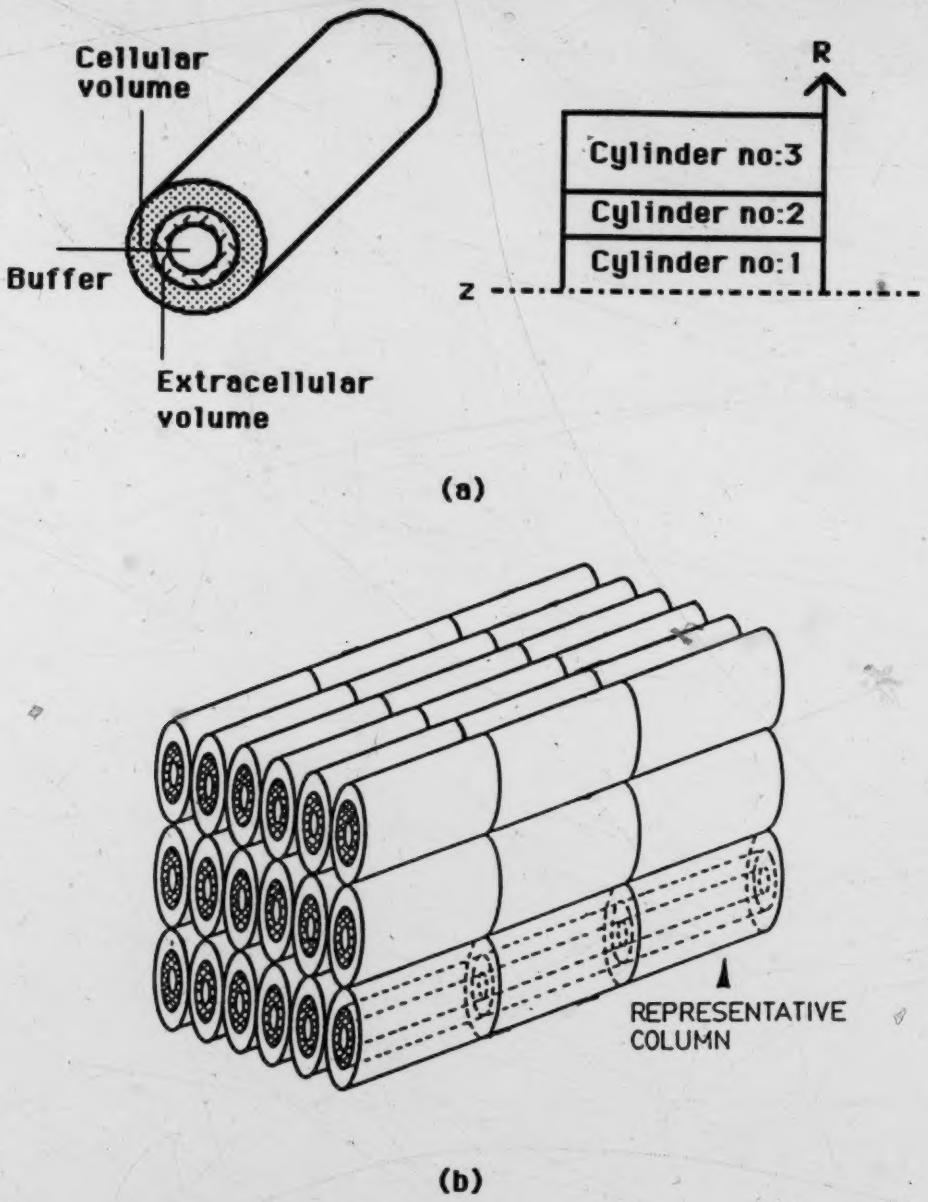
Cellular volume
Buffer
Extracellular volume
R
Cylinder no:3
Cylinder no:2
Cylinder no:1
z
(a)
REPRESENTATIVE COLUMN
(b)

Fig. 4.2 (a) Equivalent Cylindrical Unit Cell
(b) Cubic Arrangement of ECUC's.

tissue structure is approximated by an arrangement of columns. Each column is formed by a linear assemblage of ECUC.

Toupin(1986) pointed out that this representation allows for the continuity of the extracellular volume and the discontinuity of the cellular volume of the cells imposed by the tissue structure. The diffusion in the extracellular volume or apoplast transport is linearized restricting the analysis of unidirectional bulk diffusion in the tissue. Although the description of the mass transport in plant storage tissue is greatly simplified by the introduction of the ECUC concept, some geometrical transpositions are needed in order to fully describe the corresponding phenomena.

4.2 Geometrical Transposition of the Average Unit Cell into an Equilivalent Cylindrical Unit Cell

The diameter of the cellular volume, d_c, the void fraction, ϵ, which comprises the proportion in volume of the cell wall (ϕ_{cw}) and the free space (ϕ_{fs}), and the fraction of the area of the plasmalemma occupied by the plasmodesmata (αp), are available in the literature for an average unit cell of potato tissue. One can calculate the cellular volume, V_c; the extracellular or interstitium volume, V_i; and the total volume, V; as well as the total diameter of the average unit cell (d). The tortuosity (τ) of a species travelling in a porous structure of average unit cells is calculated as being the ratio of the actual distance covered as compared to the shortest physical distance. Finally, the surface area of the plasmalemma, A_m, of the average unit cell is also determined.

Based on the properties of the average unit cell, the mensurations of the equivalent cylindrical unit cell (i. e., the length, l; the radius of the buffer, R_b; the radius of the extracellular volume, R_i; the radius of the cellular volume, R_c) are calculated.

The summary of the geometrical transpositions of an average unit cell into an ECUC is shown in table 4.1. Table 4.2 reports the characteristics of both tissue. Finally fig. 4.3 shows a comparison of the existing mechanisms of mass transport into a biological structure composed of average unit cells (a) composed of equivalent cylindrical unit cells (b).

In order to model the mass transport of sucrose and water in potato tissue upon osmosis, a column of ECUC was selected as representing the entire system. The equations describing the isothermal mass transport phenomena were established. Basically, the overall bulk diffusion occuring in the extracellular space will be approached using relations associated with the extended form of second order Fick equation. The transmembrane and symplast transport will be modelled by relations based on the theory of irreversible thermodynamics. The changes occuring in the cellular volume in terms of volume and concentration of both species will be monitored on a cell-to-cell basis.

4.3 Extracellular Equations of Continuity

The following assumptions are used to model the mass transport in the extracellular cylinder:

1. Isothermal mass transport in a semi-infinite medium is considered.
2. Osmotic solutions are mixtures of water and sucrose i. e. binary system.

Table 4.1. Summary of the Geometrical Transpositions.

Average Unit Cell	Equivalent Cylindrical Unit Cell
From literature:	
d_c	
$\epsilon = \phi_{fs} + \phi_{cw}$ [4.1]	
αp	
Calculation of the Volumes: cellular, extracellular, total	Equivalent Volumes
$V_c = \dfrac{\pi d_c^3}{6}$ [4.2]	$V_c = \pi l(R_c^2 - R_i^2)$ [4.9]
$V_i = \dfrac{\epsilon V_c}{1 - \epsilon}$ [4.3]	$V_i = \pi l(R_i^2 - R_b^2)$ [4.10]
$V = V_c + V_i$ [4.4]	$V = \pi l(R_c^2 - R_b^2)$ [4.11]
Total diameter of the Cell and tortuosity	Length of the ECUC
$d = \left[\dfrac{6V}{\pi}\right]^{1/3}$ [4.5]	
	$l = d \surd \tau$ [4.12]
$\tau = \dfrac{\pi d_c}{2d_c} = \dfrac{\pi}{2}$ [4.6]	
Area of Exchange of Plasmalemma	Area of Exchange of Plasmalemma
$A_m = (1 - \alpha p)\, \pi d_c^2$ [4.7]	$A_m = 2\pi R_i l$ [4.13]
Area of Exchange of Plasmodesmata	
$Ap = A_m \alpha p/(1 - \alpha p)$ [4.8]	
	Cross-Sectional Area of Interstitium
	$A_i = \pi(R_i^2 - R_b^2)$ [4.14]

Table 4.2. Characteristics of Both Tissue.

Tissue Composed of Average Unit Cells	Tissue composed of Equivalent Cylindrical Unit Cells
$\#C = \text{INT}\left[\frac{T_t\ A_t}{V} + 1\right]$ [4.15]	$\#C_{co} = \text{INT}\left[\frac{T_t}{d} + 1\right]$ [4.16] $\#co = \frac{\#C}{\#C_{co}}$ [4.17]

A_t: cross-sectionnal area of the tissue exposed

T_t: Thickness of the tissue

V : volume of the average unit cell

d : diameter of the cell

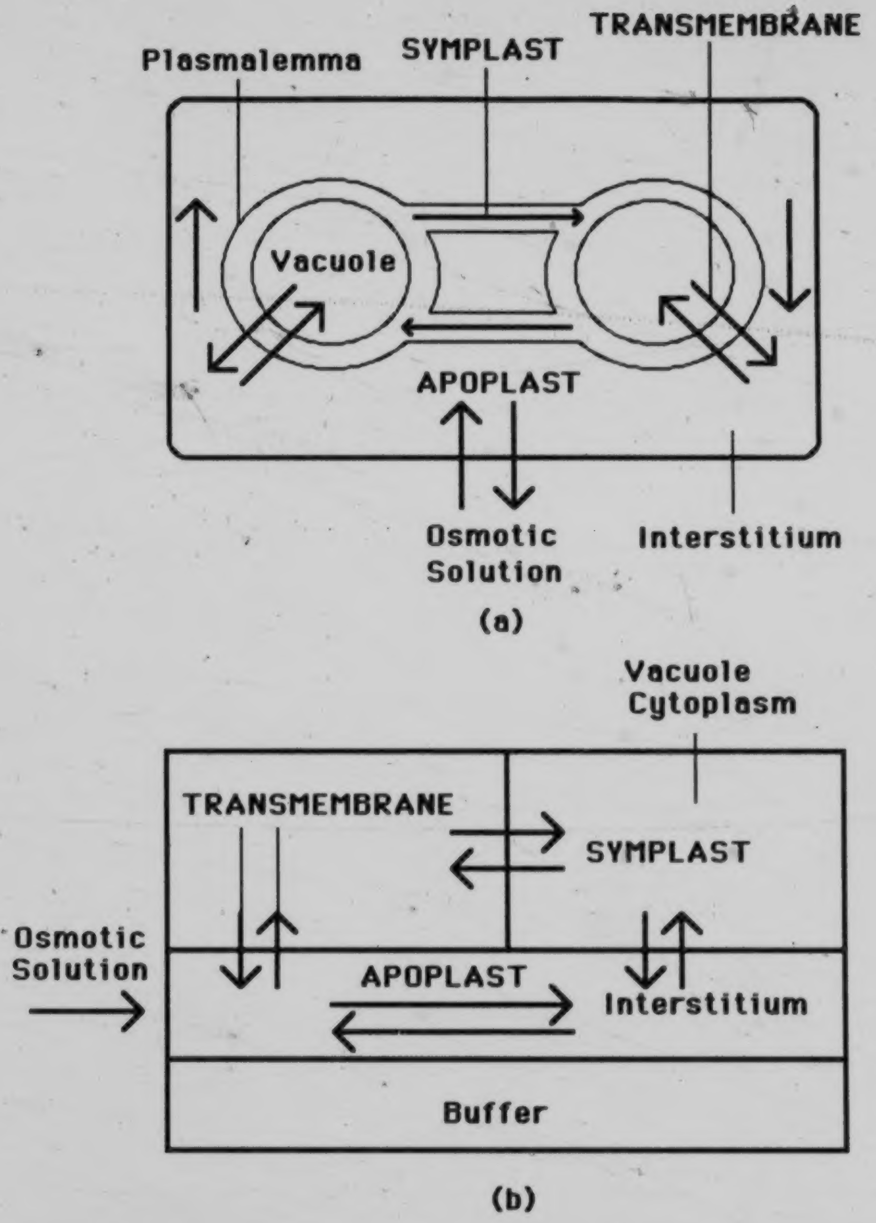
TRANSMEMBRANE
Plasmalemma
SYMPLAST
Vacuole
APOPLAST
Osmotic Solution
Interstitium
(a)
Vacuole
Cytoplasm
TRANSMEMBRANE
SYMPLAST
Osmotic Solution
APOPLAST
Interstitium
Buffer
(b)

Fig. 4.3 Comparison of the Existing Mechanisms of Transport in both Tissue Geometries (a) Average Unit Cells (b) Equivalent Cylindrical Unit Cells.

3. The space available for the sucrose to move is restricted to the extracellular volume (i. e., sucrose is impermeable to the plasmalemma membrane).
4. Water is permeable to the plasmalemma membrane.
5. Only axial diffusion occurs in the extracellular cylinder.
6. The interstitial volume as well as the cross-sectional area of transfer is either allowed to vary or not. The length, radii of the ECUC are functions of time and distance but on a cell-to-cell basis.

A differential volume element of cross-sectional area A_i is defined in the extracellular volume. Applying the law of conservation of mass, one can write a mass balance for each species: water and sucrose.

INPUT - OUTPUT + REACTION = ACCUMULATION

N is defined as a mass flux. Rwm represents the water transmembrane flux. Fig. 4.4 shows the contribution of the different fluxes in the differential volume element:

For water:

$$(A_i N_w|_z - A_i N_w|_{z+\delta z})\delta\theta + Rwm2\pi R_i\delta z\delta\theta = (A_i\rho_w|_{\theta+\delta\theta} - A_i\rho_w|_\theta)\delta z \qquad [4.18]$$

Divided by δz, $\delta\theta$,

$$\frac{(A_i N_w|_z - A_i N_w|_{z+\delta z})}{\delta z} + Rwm2\pi R_i = \frac{(A_i\rho_w|_{\theta+\delta\theta} - A_i\rho_w|_\theta)}{\delta\theta} \qquad [4.19]$$

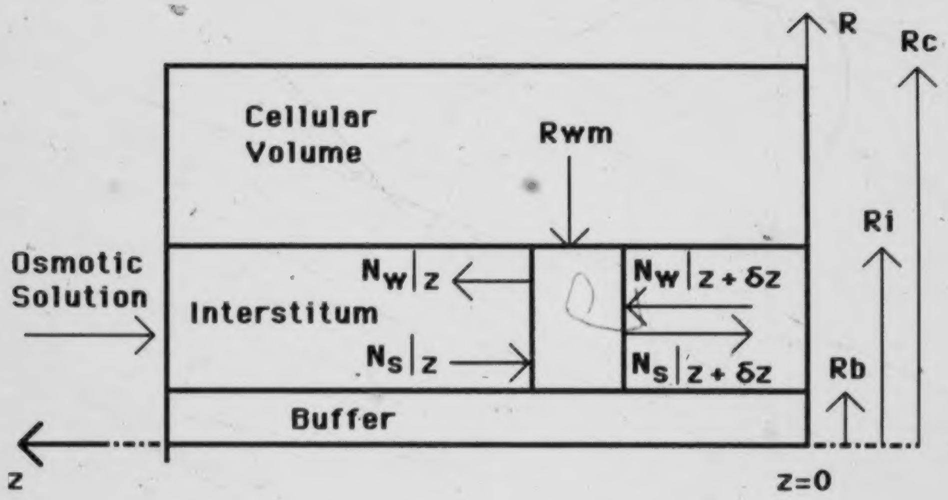
R
Rc
Cellular Volume
Rwm
Ri
Osmotic Solution
$N_w|z$
$N_w|z+\delta z$
Interstitum
$N_s|z$
$N_s|z+\delta z$
Rb
Buffer
z
z=0

Fig. 4.4 Mass Balance in a Differential Volume Element of Extracellular Space (cross-sectional area Ai) for Sucrose and Water

δz, $\delta\theta$ decrease to zero,

$$-\frac{\partial(A_iN_w)}{\partial z} + Rwm2\pi R_i = \frac{\partial(A_i\rho_w)}{\partial\theta} \qquad [4.20]$$

For sucrose,

$$-\frac{\partial(A_iN_s)}{\partial z} = \frac{\partial(A_i\rho_s)}{\partial\theta} \qquad [4.21]$$

The addition of eq.[4.20] and eq.[4.21] gives eq.[4.22] for the mixture:

$$-\frac{\partial(A_i\rho v)}{\partial z} + Rwm2\pi R_i = \frac{\partial(A_i\rho)}{\partial\theta} \qquad [4.22]$$

since;

$$\rho v = N_w + N_s \qquad [4.23]$$

Eq.[4.22] is the total equation of continuity. It utilizes the property which shows that in any mixture the sum of the relative fluxes is zero. At this stage, the choice of whether or not A_i and ρ vary with time and distance is important.

Experimentally, it was found that for a wide range of concentration of sucrose solution (10%-40%) in equilibrium with the potato material, the total volume change is the same although both the cellular and extracellular volumes are different from one concentration of osmotic solution to another. Consequently, A_i should be allowed to vary as well as 1. The geometric properties of the ECUC composing the column vary on a cell-to-cell basis. Since the cellular volume of the cells are treated as whole entities, the transfer of matter from cellular volume to the extracellular volume or vice-versa is spread equally over the entire interstitium. Furthermore, the cross-sectional area of the extracellular volume A_i is a function of time only on a cell-to-cell basis.

From appendix 6, it can be found that the change of volume due to the mixing of sucrose and water is negligible. According to Crank (1975), the behavior of a two component system satisfying the condition of zero volume change on mixing may be described in terms of a single diffusion coefficient in case of ordinary diffusion and the appropriate choice of the reference velocity which would be in this particular case the volume average velocity. Although ρ varies with the concentration of sucrose and water which change with respect to z and θ, the fluid, a solution of sucrose and water in the extracellular space, is assumed to have a constant mass density in order to simplify the problem. The variation effect of the density with the concentration of sucrose and water in the interstitium is assumed to be negligible as compared to the contribution of the transmembrane flux and the convective and diffusional fluxes. The density of the solution in the extracellular space varies between the density of water (1000kg/m^3) and the density of a 60% sucrose solution (1288.7kg/m^3).

Since it is a binary system two of the three equations (i. e., eq.[4.20], eq.[4.21] and eq.[4.22]) are independent. The equation for sucrose and the total equation of continuity will be used. The equations of continuity in the extracellular volume were developed for two particular cases.

4.3.1 Area of Extracellular Space is Fixed

Theoretically, the assumption of a fixed extracellular space is valid in the first stage of dehydration (i. e., in early osmotic dehydration processing). For each component, the equation of continuity may be written:

$$-\frac{\partial N_w}{\partial z} + \frac{Rwm2\pi R_i}{A_i} = \frac{\partial \rho_w}{\partial \theta} \qquad [4.24]$$

$$-\frac{\partial N_s}{\partial z} = \frac{\partial \rho_s}{\partial \theta} \qquad [4.25]$$

The definition of the mass flux for each component in a fixed frame of reference using the barycentric velocity (v) is:

$$N_w = J_w + \rho_w v \qquad [4.26]$$

$$N_s = J_s + \rho_s v \qquad [4.27]$$

where v is the barycentric velocity defined as follows:

$$v = \omega_s v_s + \omega_w v_w \qquad [4.28]$$

In one-dimensional system for constant ρ, the diffusional mass transfer based on the mass average velocity occurs because of a gradient in mass concentration:

$$J_w = - \mathcal{D}_w \frac{\partial \rho_w}{\partial z} \qquad [4.29]$$

$$J_s = - \mathcal{D}_s \frac{\partial \rho_s}{\partial z} \qquad [4.30]$$

The sum of the relative fluxes being zero implies that $J_w = -J_s$. There is only one independent relative flux. $\mathcal{D}_w$ and $\mathcal{D}_s$ are the diffusion coeffients with respect to the mass average velocity. The system water-sucrose solution is well documented in the literature in terms of standard diffusion coefficients (D). Yao(1981) pointed out that when dealing with diffusion problems the diffusional flux with respect to a fixed volume frame of reference is usually used and the diffusion coefficients are measured accordingly. Only in this particular case both standard diffusion coefficients are equal. Consequently, equations relating the standard solution diffusion coefficients (D) to the solution diffusion coefficients with respect to the mass average velocity were developed in appendix 7 and are listed as follows:

$$\mathcal{D}_w = \frac{DM_s}{\rho \bar{V}_s} \qquad [4.31]$$

and,

$$D_s = \frac{DM_w}{\rho \bar{V}_w} \qquad [4.32]$$

It is well known that for diffusion in a porous biological tissue the solution diffusivity has to be corrected taking into account the proportion of space available for the penetration of the solution characterized by the void fraction (ϵ). The fact that the solid matrix represents an obstacle for the solution to travel is taken into account by the tortuosity (τ).

The diffusibility is introduced to take into account the effect of the physical hindrance of the cell wall, which can affect the diffusion process in the apoplast. It is possible to characterize the resistance to diffusion in that environment using the cell wall void fraction, ϵ_{cw}, expressed as a proportion of the cell wall volume and the cell wall tortuosity, τ_{cw}, also expressed as a proportion of the cell wall volume. The diffusibility of the cell wall is defined:

$$\psi_{cw} = \frac{\epsilon_{cw}}{\tau_{cw}} \qquad [4.33]$$

The hindrance effect of the interstitium volume as a whole is a function of the combined resistances of the free space volume and the cell wall volume and is defined assuming a parallel effect:

$$\psi = (\Phi_{fs}\psi_{fs} + \Phi_{cw}\psi_{cw})/(\Phi_{fs} + \Phi_{cw}) \qquad [4.34]$$

Since there is a negligible resistance to be expected in the free space volume, the diffusibility $\psi_{fs} \cong 1$ i. e. the diffusivity is approximately the solution diffusivity.

$$\psi = (\Phi_{fs} + \Phi_{cw} - \Phi_{cw} + \Phi_{cw}\psi_{cw})/(\Phi_{fs} + \Phi_{cw}) \qquad [4.35]$$

$$\psi = \left[V_i/V - (1 - \psi_{cw})\epsilon_{cw}\right] /(V_i/V) \qquad [4.36]$$

$$\psi = 1 - [(1 - \psi_{cw})\ V_{cw}/V_i] \qquad [4.37]$$

where V_{cw} is the total volume of the cell wall comprising the voids and spaces as well as the cellulosic fibers. The cell wall volume is assumed to remain constant and is calculated from the initial total volume. V_i is the extracellular volume.

The solution diffusivities are corrected by the apparent interstitium diffusibility, ψ, so that the corrected diffusivity is defined as:

$$\bar{D}_w = \frac{\psi D M_w}{\rho \bar{V}_w} \qquad [4.38]$$

and:

$$\bar{D}_s = \frac{\psi D M_s}{\rho \bar{V}_s} \qquad [4.39]$$

where: $\bar{D}_s$ and $\bar{D}_w$: apparent diffusivity in the interstitium
D: standard solute diffusivity
ϕ: apparent diffusibility

For each component, the concentration profile is more easily described by either:

$$\frac{\partial \rho_w}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_w \frac{\partial \rho_w}{\partial z}\right] - \rho_w \frac{\partial v}{\partial z} - v\frac{\partial \rho_w}{\partial z} + Rwm\,\frac{2\pi R_i}{A_i} \qquad [4.40]$$

or;

$$\frac{\partial \rho_s}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_s \frac{\partial \rho_s}{\partial z}\right] - \rho_s \frac{\partial v}{\partial z} - v\frac{\partial \rho_s}{\partial z} \qquad [4.41]$$

and the total equation of continuity:

$$\frac{\partial v}{\partial z} = Rwm\,\frac{2\pi R_i}{A_i\,\rho} \qquad [4.42]$$

4.3.2 Area of Extracellular Space is Variable

Considering the case where the area of extracellular space is allowed to vary, it is assumed that the dehydration occurs in three stages: from full turgor to incipient plasmolysis, A_i is fixed. As soon as incipient plasmolysis is reached, A_i is variable or allowed to increase. From the equilibrium study (fig. 3.9), it can be seen that, for highly concentrated sucrose solutions (i. e., over 40% sucrose solution), the extracellular space starts to decrease when the cell volume is such that the cell looses its integrity or intrinsic properties.

$$-\frac{\partial N_w}{\partial z} + Rwm\,\frac{2\pi R_i}{A_i} = \frac{\rho_w}{A_i}\,\frac{\partial A_i}{\partial \theta} + \frac{\partial \rho_w}{\partial \theta} \qquad [4.43]$$

$$-\frac{\partial N_s}{\partial z} = \frac{\rho_s}{A_i}\,\frac{\partial A_i}{\partial \theta} + \frac{\partial \rho_s}{\partial \theta} \qquad [4.44]$$

For each component, the concentration profile is described by either:

$$\frac{\partial \rho_w}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_w\,\frac{\partial \rho_w}{\partial z}\right] - \rho_w\frac{\partial v}{\partial z} - v\frac{\partial \rho_w}{\partial z} + Rwm\frac{2\pi R_i}{A_i} - \frac{\rho_w}{A_i}\,\frac{\partial A_i}{\partial \theta} \qquad [4.45]$$

or;

$$\frac{\partial \rho_s}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_s\,\frac{\partial \rho_s}{\partial z}\right] - \rho_s\frac{\partial v}{\partial z} - v\frac{\partial \rho_s}{\partial z} - \frac{\rho_s}{A_i}\,\frac{\partial A_i}{\partial \theta} \qquad [4.46]$$

and the total equation of continuity:

$$\frac{\partial v}{\partial z} = Rwm\,\frac{2\pi R_i}{A_i\,\rho} - \frac{1}{A_i}\,\frac{\partial A_i}{\partial \theta} \qquad [4.47]$$

4.4 **Water Transmembrane Transport (Rwm)**

The term transmembrane transport (Rwm) present in the extracellular equations of continuity, indicates the mass transfer of water occurring across the plasmalemma complex. Since the membrane is fully non permeable to sucrose, only water transfer is possible.

$$Rwm = L_{wm}\ \Delta\mu_{wm} \qquad [4.48]$$

where L_{wm} is the phenomenological coefficient for a water chemical potential driving force through the plasmalemma membrane. $\Delta\mu_{wm}$ is the difference in chemical potential of water across the membrane:

$$\Delta\mu_{wm} = \mu_{wm}^{in} - \mu_{wm}^{out} \qquad [4.49]$$

where μ_{wm}^{in} is the chemical potential of water inside the cellular volume and μ_{wm}^{out} is the water chemical potential of the extracellular volume with respect to the same reference state and finally $\Delta\mu_{wm}$ is the difference in chemical potential across the membrane.

Only the transport of non-electrolytes is considered. Pure free water at atmospheric pressure (P^o) and constant temperature is chosen as a reference state. The general expression for the chemical potential of water is:

$$\mu_w = \mu_w^o + \mathbb{R}T \ln \hat{a}_w + \bar{V}_w\varphi_m + \bar{V}_w(P - P^o) \qquad [4.50]$$

$\mathbb{R}T \ln \hat{a}_w$, or osmotic potential, reflects the contribution of dissolved solutes to the chemical potential of water. $\bar{V}_w\varphi_m$, or matric potential, arises because of the strong interactions between water and solids of large surface area present in the system. $\bar{V}_w(P - P^o)$, or pressure potential, expresses the dependence of the water chemical potential on hydrostatic pressure.

The extracellular volume is composed of the free space and the cell wall which are usually filled with air. However any pretreatment, such as transferring disks of biological material in distilled water and storing them not only ensure that the tissue is initially at full turgor but also that the intercellular spaces and cell wall volumes are likely to be water filled. Sucrose penetrates in the extracellular volume as the osmotic treatment is pursued contributing more and more to the osmotic potential of the extracellular space. The hindrance effect of the wall has been taken into account with the diffusibility (ψ) value. The interactions between the cellulose matrix and the solution are assumed to be negligible so that the matric potential contribution in the extracellular space is considered negligible. The pressure potential term is zero, since the extracellular medium is directly in contact with an osmotic solution open to the atmosphere. Thus the chemical potential of water in the extracellular space is simply:

$$\mu_{wm}^{out} - \mu_{wm}^{out^{o}} = \mathbb{R}T \ln \hat{a}_{wfs} \qquad [4.51]$$

$\mathbb{R}T \ln \hat{a}_{wfs}$ reflects the increasing contribution of the sucrose penetrating the extracellular space during the osmotic treatment. $\hat{a}_{wfs}$ is calculated by:

$$\hat{a}_{wfs} = \gamma_w \, x_w \qquad [4.52]$$

where γ_w is the activity coefficient of water and x_w is the mole fraction of water.

A correlation was made between the activity coefficient, γ_w, and the mole fraction of sucrose (x_s) using the data of Morris from Hougen and Watson(1954) at 25°C. It was found that:

$$\ln \gamma_w = - x_s^2(3.36 + 90.5\ x_s - 623.6\ x_s^2) \qquad [4.53]$$

The correction for the temperature was also applied:

$$a_{wfs}^{40} = a_{wfs}^{25} \exp\ (0.0004979\ m_s^2) \qquad [4.54]$$

where m_s is the molality of sucrose.

The experimental measurements of the equilibrium study have shown that, in the case of an osmotic treatment with an aqueous solution of an impermeable solute, such as sucrose, the mass and volume changes of the cellular volume as well as the concentration of the different components inside the cellular volume of the potato cell are fully described by considering the water chemical potential of the different phases present. The cellular volume includes the vacuole and the cytoplasm which comprises starch and proteins. The pressure potential is calculated on a cellular volume basis. If we assume that the cellular volume is in equilibrium with the extracellular volume:

$$\mu_{wm}^{out} - \mu_{wm}^{out^o} = \mu_{wm}^{in} - \mu_{wm}^{in^o} + \overline{V}_w(P_c - P_c^o) \qquad [4.55]$$

The pressure potential is defined as:

$$\bar{V}_w(P_c - P_c^o) = \bar{V}_w \left[\left[\left[\frac{V_c}{V_c^{ft}}\right]^{\beta_1} \left[P_c^{ft} + \frac{\beta_2}{\beta_1}\right]\right] - \frac{\beta_2}{\beta_1}\right] \qquad [4.56]$$

where P_c^{ft} is defined as the excess of pressure above the atmospheric pressure at full turgor. The reader is referred to section 3.2.1.3.1 for details. V_c/V_c^{ft} represents the ratio of the actual cellular volume over the cellular volume at full turgor. β_1 and β_2 are the literature values for potato tissue which describe the variation of the elastic modulus of the cell wall (ξ) as a function of the turgor pressure.

At the vacuole phase the osmotic potential is important. Since the vacuole aqueous solution is composed of small amount of minerals and soluble sugars. These solutes contribute to the osmotic potential. For multicomponent systems, a relationship between the partial water activity of each component and the water activity of the mixture was derived by Ross(1975) considering that all water present in the system forms a solution with each of the components independently of each other. Thus:

$$\mu_{wm}^{in} - \mu_{wm}^{in^o} = RT \ln \hat{a}_{wv} = RT \ln \left[\prod_j \hat{a}_{wj}\right] \qquad [4.57]$$

On the basis of equivalent binary water-j component:

$$\hat{a}_{wj} = 10^{-\Lambda_j(1 - x_{wj})^{q_j}} x_{wj} \qquad [4.58]$$

The water mole fraction:

$$x_{wj} = \frac{X_v}{X_v + w_j \alpha_j} \qquad [4.59]$$

where:

$$\alpha_j = \frac{M_w}{M_j} \qquad [4.60]$$

The values of Λ and q are available in table 3.10.

At the cytoplasm phase, since starch and the proteins are the major components the matric potential is dominant. Empirical correlations for sorption isotherms of starch and proteins are given by Crapiste and Rotstein(1982) and used to estimate the matric potential.

$$\mu_{wm}^{in} - \mu_{wm}^{in^o} = \mathbb{R}T \ln \left[1 - \exp(53.4759 \, X_{st}^{2.3015} \right] \qquad [4.61]$$

$$\mu_{wm}^{in} - \mu_{wm}^{in^o} = \mathbb{R}T \ln \left[-0.0208 \, X_{pr}^{-1.6129} \right] \quad . \qquad [4.62]$$

As we can see the chemical potential inside the cellular volume, $\mu_{wm}^{in} - \mu_{wm}^{in^o}$, can be estimated either from the vacuole phase contribution or from the cytoplasm phase contribution, since the chemical potential of both phases was assumed to be equal.

Since $\mu_{wm}^{in^o} = \mu_{wm}^{out^o}$, $\Delta\mu_{wm}$ is defined by either:

$$\Delta\mu_{wm} = \bar{V}_w(P_c - P_c^o) + \mathbb{R}T \ln \hat{a}_{wv} - \mathbb{R}T \ln \hat{a}_{wfs} \qquad [4.63]$$

or;

$$\Delta\mu_{wm} = \bar{V}_w(P_c - P_c^o) + \mathbb{R}T \ln\left[1 - \exp\left[-53.4759\, X_{st}^{2.3015}\right]\right]$$

$$+ \mathbb{R}T \ln\left[-0.0208\, X_{pr}^{-1.6129}\right] - \mathbb{R}T \ln \hat{a}_{wfs} \qquad [4.64]$$

Thus the flux of water across the membrane is expressed by either:

$$Rwm = L_{wm}\left[\mathbb{R}T \ln \frac{\hat{a}_{wv}}{\hat{a}_{wfs}} + \bar{V}_w(P_c - P_c^o)\right] \qquad [4.65]$$

or;

$$Rwm = L_{wm}\left[\bar{V}_w(P_c - P_c^o) + \mathbb{R}T \ln\left[1 - \exp\left[-53.4759\, X_{st}^{2.3015}\right]\right]\right.$$

$$\left. + \mathbb{R}T \ln\left[-0.0208\, X_{pr}^{-1.6129}\right] - \mathbb{R}T \ln \hat{a}_{wfs}\right] \qquad [4.66]$$

From the literature the permeability coefficient of the plasmalemma membrane, $\mathcal{P}_{wm}$, can be found (Rotstein and Cornish, 1978a):

$$L_{wm} = \frac{\mathcal{P}_{wm}\, M_w}{\mathbb{R}T\, \bar{V}_w} \qquad [4.67]$$

μ_{wm}^{out} varies with the position in the extracellular space whereas μ_w^{in} varies but on a cell-to-cell basis.

4.5. Intracellular Equations of Change

In the description of the volume and concentration changes in the cellular volume, the following assumptions were considered:

1. Perfect mixing in the cellular volume.
2. The plasmalemma surface area is fixed.
3. Equations are established on a cell-to-cell basis.
4. The symplastic transport was not considered in the present study.

The contributions to the variation of the mass concentration of species present in the cellular volume are function of the water loss from the cellular volume through the membrane. If the symplastic transport is considered negligible the cells behave as if they were independent. For each cellular volume, one can write specifically a mass balance:

$$- \delta\theta \; 2\pi R_i \int^{c} Rwm \; dz = m_w^c \Big|_{\theta+\delta\theta} - m_w^c \Big|_{\theta} \qquad [4.68]$$

The concentration of water in the cellular volume is expressed in terms of total moisture content (X) on a dry matter basis which is convenient since a dehydration process takes place in the cellular volume. The total moiture content on a dry matter basis is related to the moisture content (m_w) with the mass of dry matter (m_{dm}).

$$- \delta\theta \; 2\pi R_i \int^{c} Rwm \; dz = X \; m_{dm} \Big|_{\theta+\delta\theta} - X \; m_{dm} \Big|_{\theta} \qquad [4.69]$$

After dividing by $\delta\theta$ and taking the limit as $\delta\theta$ tend to zero one obtains:

$$\frac{dX}{d\theta} = - \frac{2\pi R_i}{m_{dm}} \int^{c} Rwm \; dz \qquad [4.70]$$

The mass of dry matter of the cellular volume is estimated from the composition of the phases included in the cellular volume of the potato tissue and the volume of the intracellular volume of the fresh potato assuming that the density of the cellular volume approaches the density of water.

The cellular volume variation is a function of the volume of water loss through the transmembrane on a cell-to-cell basis. Neglecting the change of volume on mixing:

$$\frac{dV_c}{d\theta} = - \frac{2\pi R_i}{M_w} \int^{c} \bar{V}_w \, Rwm \; dz \qquad [4.71]$$

In order to estimate the complete composition X_v, X_{st} and X_{pr}. A test is made in order to see if the pressure potential term exists. Eq.[4.56] is used to calculate the pressure potential term. Knowing X, the moisture content in the cellular volume on a dry matter basis, a first guess for the water chemical potential inside the cellular volume is calculated from the Hasley(1948) correlation (i. e., eq.[3.39]). The moisture content of the starch (X_{st}) and proteins (X_{pr}) are calculated using eq.[4.61] and eq.[4.62]. By difference the moisture of the vacuole is estimated:

$$X_v = X - X_{st}w_{st} - X_{pr}w_{pr} \qquad [4.72]$$

The water activity of the vacuole phase is determined using eq.[4.57], eq.[4.58], eq.[4.59] and eq.[4.60]. Since there is an equality between the chemical potential of water in the vacuole and the cytoplasm, the water chemical potential obtained from the vacuolar composition is compared with the guess on the water chemical potential obtained from the total moisture content until convergence on proper value of the new chemical potential of water inside the cellular volume ($\mu_{wm}^{in} - \mu_{wm}^{in^o}$) corresponding to the proper composition of the phases.

4.6 Geometrical Time Derivative Relations

In the development of the model, geometrical relations were used to evaluate the equivalent cylindrical unit cell mensurations. The geometrical equations of change are time derivative on a cell-to-cell basis.

$$\frac{dV_i}{d\theta} = \kappa \frac{dV_c}{d\theta} \qquad [4.73]$$

and,

$$\frac{dV}{d\theta} = (1 + \kappa) \frac{dV_c}{d\theta} \qquad [4.74]$$

The compliance factor κ describes how cellular volume changes affect the extracellular volume of the cell. From full turgor to incipient plasmolysis $\kappa = 0$ which represents the fact that the total volume decreases as the cellular volume decreases. The extracellular volume is assumed to be constant. As soon as the pressure potential is zero, $\kappa = -1$ (i. e., plasmolysis has occured). The total volume is kept constant. The extracellular volume increases as much as the cellular volume decreases. Finally, a loss of the integrity of the cell seems to occur as the ratio of the actual cellular volume over the cellular volume at full turgor reaches 0.3 (fig. 3.9), particularly for highly concentrated sucrose solution (i. e., over 40% sucrose solution). Consequently, $\kappa = 1$ which characterizes the fact that the cellular volume decreases as much as the extracellular volume. The geometrical relations of the ECUC are listed in table 4.3.

4.7 Initial and Boundary Conditions

4.7.1 Initial Conditions

The initial conditions in the representative column of ECUC are presented for $\theta = 0$ as follows:

1. For all cells i. e. cj=1, #C: $R_b^{cj} = R_b^o$; $R_i^{cj} = R_i^o$; $R_c^{cj} = R_c^o$; $l^{cj} = l^o$; $A_m^{cj} = A_m^o$; $A_i^{cj} = A_i^o$; $V_c^{cj} = V_c^o$; $V_i^{cj} = V_i^o$; $V^{cj} = V^o$; $\psi^{cj} = \psi^o$.

2. For all cells i. e. cj=1, #C: $X^{cj} = X^o$; $X_v^{cj} = X_v^o$; $X_{st}^{cj} = X_{st}^o$; $X_{pr}^{cj} = X_{pr}^o$.

3. In the interstitium for any point, $\rho_s^j = \rho_s^o$

Table 4.3. Geometrical Time Derivative Relations of the ECUC.

$$\frac{dl}{d\theta} = \frac{\sqrt{\tau}}{3} \left[\frac{6}{\pi}\right]^{1/3} V^{-2/3} \frac{dV}{d\theta} \qquad [4.75]$$

$$\frac{dR_i}{d\theta} = - \frac{A_m}{2\pi} l^{-2} \frac{dl}{d\theta} \qquad [4.76]$$

$$\frac{dR_c}{d\theta} = \frac{1}{2\pi R_c} \left[l^{-1} \frac{dV_c}{d\theta} - V_c l^{-2} \frac{dl}{d\theta}\right] + \frac{R_i}{R_c} \frac{dR_i}{d\theta} \qquad [4.77]$$

$$\frac{dR_b}{d\theta} = \frac{R_i}{R_b} \frac{dR_i}{d\theta} - \frac{1}{2\pi R_b} \left[l^{-1} \frac{dV_i}{d\theta} - V_i l^{-2} \frac{dl}{d\theta}\right] \qquad [4.78]$$

$$\frac{d\psi}{d\theta} = (1 - \psi_{cw}) \frac{V_w}{V_i^2} \frac{dV_i}{d\theta} \qquad [4.79]$$

$$\frac{dA_i}{d\theta} = 2\pi \left[R_i \frac{dR_i}{d\theta} - R_b \frac{dR_b}{d\theta}\right] \qquad [4.80]$$

4. Assuming that the tissue is initially in equilibrium with pure water i. e. there is no symplast transport (Rwp = 0), no transmembrane transport (Rwm = 0) or apoplast (N_w, Ns) i. e. v = 0, $\frac{dv}{dz} = 0$ at $\theta = 0$.

4.7.2 Boundary Conditions

Three locations are considered: the surface of the tissue, the center and the interface between two adjoining cells.

4.7.2.1 Surface of the Tissue

Assuming that there is no resistance to mass transfer at the surface of the biological structure, the concentration of sucrose in the interstitium at the surface is equal to the concentration of sucrose of the bath solution or osmotic solution. For a system under a vigorous agitation, the assumption is justified:

$$\rho_s\big|_s = \rho_{sos} \tag{4.81}$$

4.7.2.2 Center of the Tissue

Considering a semi-infinite medium, the center is defined as a plane parallel to the surface situated at a distance equal to the thickness of the tissue. For any point located on that plane and beyond, the extracellular and cellular conditions remain at any time equal to the initial conditions, $\theta = 0$:

$$\rho_s\big|_o = \rho_s^o \tag{4.82}$$

Since the intracellular equations of change are defined with respect to the mass of dry matter:

$$X\big|_o = X^o \qquad [4{:}83]$$

For all species, there is no symplast transport $(Rwp\big|_o = 0)$, no apoplast transport i. e. $\frac{dv}{dz}\Big|_o$ and $v\big|_o$ equal zero.

4.7.2.3 Interface Between Two Adjoining Cells

The major consequence of describing the behavior of the representative column on a cell-to-cell basis is that it creates discontinuities at the interface between 2 adjoining cells. A special analysis of mass transfer is required to link the transport phenomena occurring in the interstitium of each cell at the interface. Specifically for sucrose:

$$A_i\, N_s\big|_{cj,in} = A_i\, N_s\big|_{cj+1,in} \qquad [4.84]$$

Eq.[4.89] states that there is conservation of mass for both species sucrose and water in the interstitium at the interface.

If $\rho_{s_{cj,in}} = \rho_{s_{cj+1,in}}$ the convective transfer:

$$\left[A_i v\right]_{cj,in} = \left[A_i v\right]_{cj+1,in} \qquad [4.85]$$

Same Treatment for sucrose leads to:

$$\left[A_i \, \bar{D}_s \, \frac{\partial \rho_s}{\partial z} \right]_{cj,in} = \left[A_i \, \bar{D}_s \, \frac{\partial \rho_s}{\partial z} \right]_{cj+1,in} \qquad [4.86]$$

These relations allow for the mergence of the information pertaining to each of the two interface points into a unique quantity, therefore eliminating the need to use an extended space grid in solving the equations of the extracellular space.

4.8 **Summary of the Equations and Description of the Numerical Method**

Table 4.4 summarizes the analysis of the section 4 by presenting the list of the model equations.

The equation describing the mass transport of species in the extracellular space is a function of time and distance. This partial differential equation (PDE) is parabolic and highly non linear since D, ψ, v, $\frac{\partial v}{\partial z}$, $\frac{\partial A_i}{\partial \theta}$ are implicitly function of the interstitium concentration of sucrose.

The intracellular equations of change i. e. the cellular volume, the extracellular volume, the total volume and the water concentration of the cellular volume, as well as the geometrical relations form a system of ordinary differential equations (ODE) on a cell-to-cell basis. These equations are function of time only.

The integration of the transmembrane fluxes over the entire cell requires the fitting of discrete values of transmembrane fluxes and the calculation of the surface under the resulting curve over each cellular volume in order to obtain the mass average velocity.

Table 4.4. Summary of the Model Equations.

Description	Equation number
Extracellular Equation of Continuity	
1) Area (A_i) is fixed	
-Sucrose	[4.41]
-Total	[4.42]
2) Area (A_i) is variable	
-Sucrose	[4.46]
-Total	[4.47]
Transmembrane Transport (Rwm)	[4.65] or [4.66]
$-\mu_{wm}^{out} - \mu_{wm}^{out^o}$	[4.51], [4.52], [4.53] [4.54]
$-\mu_{wm}^{in} - \mu_{wm}^{in^o}$	
- Pressure Term	[4.56]
- Osmotic Potential Term	
either	[4.58], [4.59], [4.60]
or	[4.61], [4.62]
$-L_{wm}$	[4.67]
Intracellular Equations of Change assuming that the symplast is negligible	
-Total Moisture Content	[4.70]
-Cellular Volume	[4.71]
Geometrical Time Derivative Relations	[4.73] - [4.80]
Initial Conditions	Section 4.7.1
Boundary Conditions	
-Surface of the Tissue	[4.81]
-Center of the Tissue	[4.82], [4.83]
-Interface between two Cells	[4.85], [4.86]

These relations are integrated numerically in order to obtain the transient concentration profile.

The methods available for solving nonlinear parabolic differential equations are limited. Generally a discretization both in time (θ)and position(z) is performed. An implicit scheme such as Crank-Nicolson (CN) has been chosen. Theoretically the CN is unconditionnally stable. Since it has been developed for a similar system (Toupin, 1986) with many interesting features, it was modified for this particular system. Details on the development of Crank Nicolson are available in appendix 8. Because of the non linearity of the terms an iteration procedure is required to solve for the transient concentration profile. A projection to half level in time is performed followed by an evaluation of the non linear terms. An estimate of the concentration profile is obtained at the next time level. An iteration is pursued until convergence on the concentrations at the next time level is reached within the limit of the tolerance.

In order to perform the integration of the system of ordinary differential equations (ODE), a simple discretization was performed with respect to time. Even though the gradients generated in the extracellular volume are important with respect to the distance variable, the effect is considerably reduced with respect to time particularly on a cell-to-cell basis. Consequently, the ordinary differential equations are smooth and the time dependent variables change slowly.

4.9 Results of the Simulations

4.9.1 Testing the Numerical Method

Assuming a pure diffusion phenomenon in the extracellular space, the Crank-Nicolson scheme was tested by comparing the numerical sucrose concentration profile to the analytical solution of the second order Fick's law of diffusion. For a semi infinite medium:

$$\frac{\rho_s - \rho_s^o}{\rho_{sos} - \rho_s^o} = \mathrm{erfc}\left[\frac{z}{2\sqrt{D\theta}}\right] \qquad [4.94]$$

where ρ_{sos} is the sucrose concentration of the osmotic solution. The mass transfer coefficient at the surface was assumed to be infinite and the diffusivity assumed to remain constant. Simulations were carried out for different number of grid points. It was found that a minimum of 7 points per cell was sufficient for the numerical concentration profile to match the analytical concentration profile with a $\Delta\theta$ varying from 5 to 20 seconds. Convergence is better achieved with a $\Delta\theta$=5s although after 120s the sucrose concentration profile for $\Delta\theta$ varying between 5 and 20 seconds matches the analytical profile. It is important to keep a sufficient number of points in order to be able to carry out properly the spline fitting and integration of the transmembrane fluxes over the entire cell. $D\Delta\theta/(\Delta z)^2$ was calculated for $\Delta\theta$=5s, 10s and 20s. It was found that, for $\Delta\theta$=5s, $D\Delta\theta/(\Delta z)^2$=1.87, for $\Delta\theta$=10s, $D\Delta\theta/(\Delta z)^2$=3.74 and for θ=20s, $D\Delta\theta/(\delta z)^2$=7.47. In order to keep a reasonable $\Delta\theta$ (i. e., at least 5s), an implicit scheme must be used since the condition of stability for an explicit scheme is $D\Delta\theta/(\Delta z)^2$ has to be smaller or equal to 0.5. The importance of using an implicit scheme is clearly shown here.

The variation of the diffusion with the sucrose concentration was introduced in the model to test the effect of the non linearity of the diffusion coefficient on the numerical profile. Same $\Delta\theta$ and number of grids ensured proper convergence on the sucrose concentration profile. A $\Delta\theta$ of 5s was selected for the first 10 seconds of simulation then for the next 10 seconds of simulation a $\Delta\theta$ of 10s was used and finally a $\Delta\theta$ of 20s was used for all other time with 7 grids in order to minimize the computation time but to ensure the proper convergence on the sucrose concentration profile.

As mentioned before, an iteration procedure is used to get the sucrose concentration profile. A projection is made at half time level to evaluate the non linear terms. The calculation of the sucrose concentration at the next time level is pursued. The convergence on the proper sucrose concentration profile is achieved if the difference between two consecutive values of concentration at the next time level is less than 0.001 for the first 600s and 0.01 for all other time at each grid point. This was found to be sufficient with respect to the experimental error on the measurement of sucrose content. A maximum a 20 iterations was allowed for the convergence to be reached.

In order to be able to assume a semi infinite medium as a geometry, the concentration at the centre has to remain the same as the initial value throughout the simulation. Based on the experimental data, a thickness of tissue exposed of 5×10^{-3} m to 6×10^{-3} m seemed to be sufficient. An estimation of the limiting thickness was also made considering a simple diffusion after 1 hour treatment in a 60% sucrose solution. A value of the reduced concentration $\frac{\rho_s - \rho_s^0}{\rho_{sos} - \rho_s^0}$ of 0.0001 was considered negligible. The diffusivity coefficient was assumed to be the one at infinite dilution. It was found that a thickness of 6.3×10^{-3} m would be sufficient to ensure that the sucrose concentration at the centre remain unchanged. Consequently, the simulations were performed with a 6.4×10^{-3} m thickness.

4.9.2 Symplasm is not Present and Variable Surface Area of Extracellular Space is Considered

The values of the parameters required by the model are listed in table 4.5. They were obtained partly from the literature and partly from the results of the experimental work.

The simulations were carried out to test the appropriateness of the model by comparing predicted and experimental observations. The conditions of the potato material immersed in a 60% sucrose solution for 1 hour were considered. From the results of the equilibrium and the kinetic studies, it was found that the surface area of extracellular space varies quite dramatically. Furthermore the variation of the extracellular space was included. However, the symplastic transport was not taken into account.

Fig. 4.5 shows the sucrose concentration profile in the extracellular space for a 1 hour treatment in a 60% sucrose solution. The solid line curve represents the sucrose concentration profile considering only a simple diffusion in the extracellular space with a variable diffusion coefficient which varies with the sucrose

Table 4.5 Summary of the Parameter Values used for the Simulations of an Osmotic Treatment of Potato Tissue in a 60% Osmotic Solution for 1 hour.

Description	Units	Values
Osmoticum Characteristics		
-Temperature	oC	40
-Partial Molar Volumes	m3/kmol	
water		0.018016
sucrose		0.211
-Molecular Weights	kg/kmol	
water		18.0
sucrose		342.3
-Diffusivity of Sucrose in Water		
D^{∞}	m2/s	7.53×10^{-10}
a_0		
a_1	kg/m3	-0.0020882
Initial Tissue Characteristics		
-Thickness	m	5.0×10^{-3}*
-Surface Area Exposed	m2	0.000157
-Cell Wall Volume Fraction	ϕ_{cw}	0.01
-Free Space Volume Fraction	ϕ_{fs}	0.03
-Tortuosity		1.57
-Interstitium Sucrose Concentration	kg/m3	0.0

* Although the thickness of the tissue exposed is 5×10^{-3}m, the thickness of the equivalent tissue geometry is 6.4×10^{-3}m.

Table 4.5(cont'd)

Initial Cell Characteristics		
-Cell Diameter	m	1.80×10^{-4}
-Cell Wall Diffusibility		0.3
-Elastic Modulus (ξ)		
β_1	—	3.5
β_2	Pa	0.5×10^{6}
-Turgor Pressure	Pa	$0.5\mathrm{X}10^{6}$
-Membrane Permeability (P_{wm})	m/s	0.34×10^{-6}
or varying from		0.425×10^{-6}
to		4.25×10^{-6}
-Cell Composition on a Dry Matter Basis		table 3.9
-Cell Water Content on a Dry Matter Basis		
X	kgwater/kgdrymatter	5.4578
X_{st}	kgwater/kgdrystarch	0.3769
X_{pr}	kgwater/kgdryproteins	3.0238
X_v	kgwater/kgdrymatter	4.8689
-Density of Dry Matter	kg/m3	1613
-Density of Water	kg/m3	992.4
-Molecular Weights	kg/kmol	
K_3PO_4		212
K_2SO_4		174
Glucose		180
Fructose		180

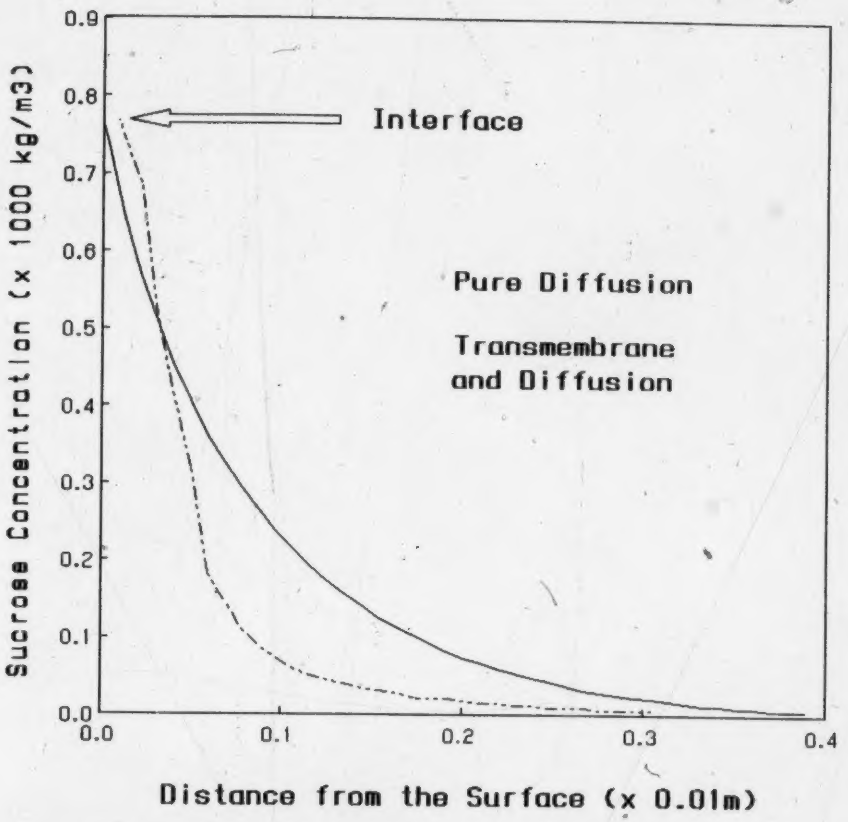

Fig 4.5 Sucrose Concentration Profile in the Extracellular Space for a 1 hour Osmotic Treatment in a 60% Sucrose Solution.

concentration. The second curve shows not only the contribution of the diffusional flux but also the contribution of the transmembrane flux in the extracellular space. The effect of including the transmembrane flux sharpens the sucrose concentration profile. The water coming out from the cellular volume through the plasmalemma membrane has restricted the sugar penetration in the extracellular space. It is also interesting to note that the interface or surface of the tissue has moved from its original value. This represents the shrinkage behavior that is observed experimentally. The cellular volume has lost some water through the plasmalemma membrane and has shrunk accordingly particularly the surface cell.

4.9.3 **Comparison between the Predicted and Experimental Values of Sucrose and Water Content**

In order to compare the predicted values to the experimental values, some data transformations have been made on the predicted values. ρ_s which represents the sucrose concentration in the extracellular volume and X which represents the water concentration in the cellular volume are predicted by the model as well as the total volume, V, the extracellular volume, V_i, and the cellular volume, V_c of the potato cell. The average sucrose concentration in the extracellular space attached to a cell is defined as:

$$\bar{\rho}_s = \frac{1}{\Delta z} \int^{c} \rho_s dz \qquad [4.95]$$

As well the water concentration:

$$\rho_w = \rho - \bar{\rho}_s \qquad [4.96]$$

where ρ is an average between the density of the liquid of the extracellular space of the potato tissue initially and the density of a 60% sucrose solution. The sucrose concentration in the cellular volume is defined as:

$$\rho_s^c = \frac{w_s}{\dfrac{X}{\rho_w^*} + \dfrac{1}{\rho_{dm}^*}} \qquad [4.97]$$

and,

$$\rho_w^c = \frac{X}{\dfrac{X}{\rho_w^*} + \dfrac{1}{\rho_{dm}^*}} \qquad [4.98]$$

The mass of the cellular volume:

$$m_c = (X + 1)\ m_{dm} \qquad [4.99]$$

where m_{dm} is estimated from the initial cellular volume V_c^o, the density of water ρ_w and the proportion of dry matter in the cellular volume 18% for the fresh material (table 3.1) but 13% for the full turgor material.

$$m_{dm} = V_c^o \times 0.13 \ / \ \rho_w \qquad [4.100]$$

The mass of extracellular volume is calculated by:

$$m_i = \rho V_i + m_{cel} \qquad [4.101]$$

where m_{cel} represents the mass of cellulose:

$$m_{cel} = V_i^o \times 0.04 / \rho_w \qquad [4.102]$$

The weight fraction of sucrose in the tissue is defined as:

$$\omega_s = \frac{\overset{\Delta z}{\Sigma} \left[\bar{\rho}_s V_i + \rho_s^c V_c\right]}{\overset{\Delta z}{\Sigma} \; (m_i + m_c)} \qquad [4.103]$$

The summation is performed over the thickness, Δz, corresponding to the experimental thickness of the slice. Please note, that the thickness may involve part of the whole cell. In the same way, the weight fraction of water of the tissue is defined as:

$$\omega_w = \frac{\overset{\Delta z}{\Sigma} \left[\rho_w V_i + \rho_w^c V_c\right]}{\overset{\Delta z}{\Sigma} \; (m_i + m_c)} \qquad [4.104]$$

The weight fraction of sucrose was also calculated assuming only a simple diffusion phenomenon in the whole tissue (i.e., the transmembrane flux was not considered). The diffusion coefficient was assumed to vary with the sucrose concentration. Since the sucrose concentration profile is shown on fig. 4.5, for a diffusion phenomenon only, the weight fraction of sucrose in the tissue is defined as:

$$\omega_s = \frac{\rho_s}{\rho} (1 - \omega_{dm}) \qquad [4.105]$$

where ω_s represents the weight fraction of sucrose in the tissue, ρ_s is the predicted volumetric concentration of sucrose in the tissue, ρ is an average value of the density between the density of a 60% sucrose solution and the density of the potato initially (1.144505), ω_{dm} is the initial weight fraction of dry matter (i. e., 15% at full turgor).

The predicted weight fraction of sugar was compared with the experimental values from the kinetic study in fig. 4.6. Different values of permeabilities were used to carry out the simulations. The small dash line indicated that the value of the permeability coefficient was fixed to $0.34\text{x}10^{-6}$m/s and that two stages of dehydration were considered. The large dash line assumed a variable permeability coefficient defined as:

$$L = 4.25\text{x}10^{-4} \exp(-3.0\rho_s) \qquad [4.106]$$

Three stages of dehydration were also assumed.

Fig.4.7 shows the comparison between the predicted water content and the experimental values from the kinetic study for different values of permeabilities.

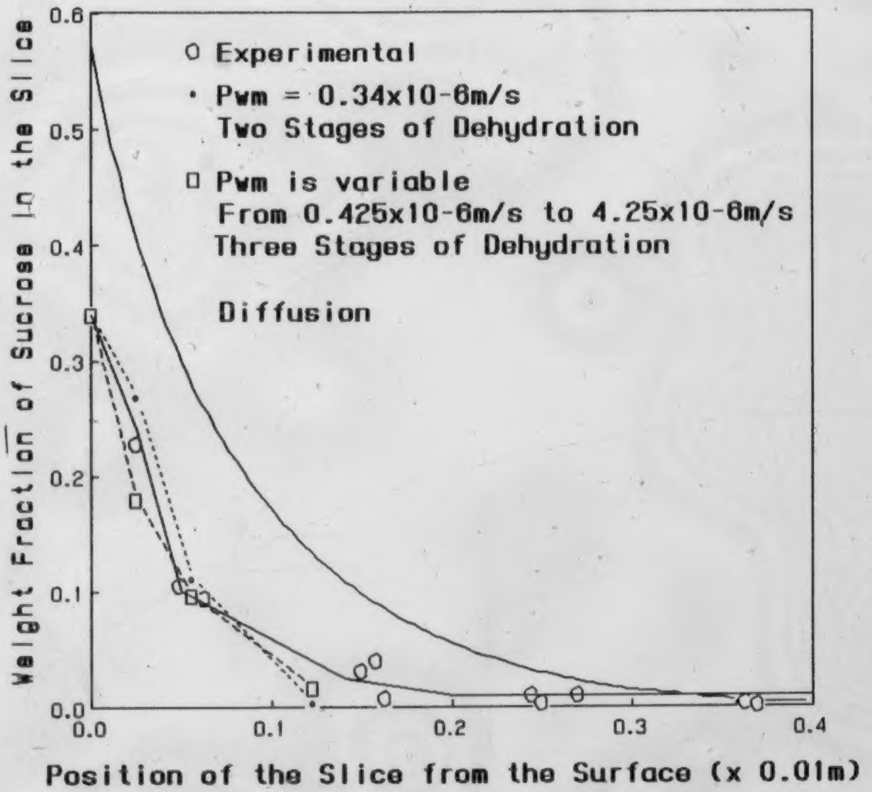

Fig. 4.6 Comparison between the Experimental and Predicted Values of Sucrose Content.

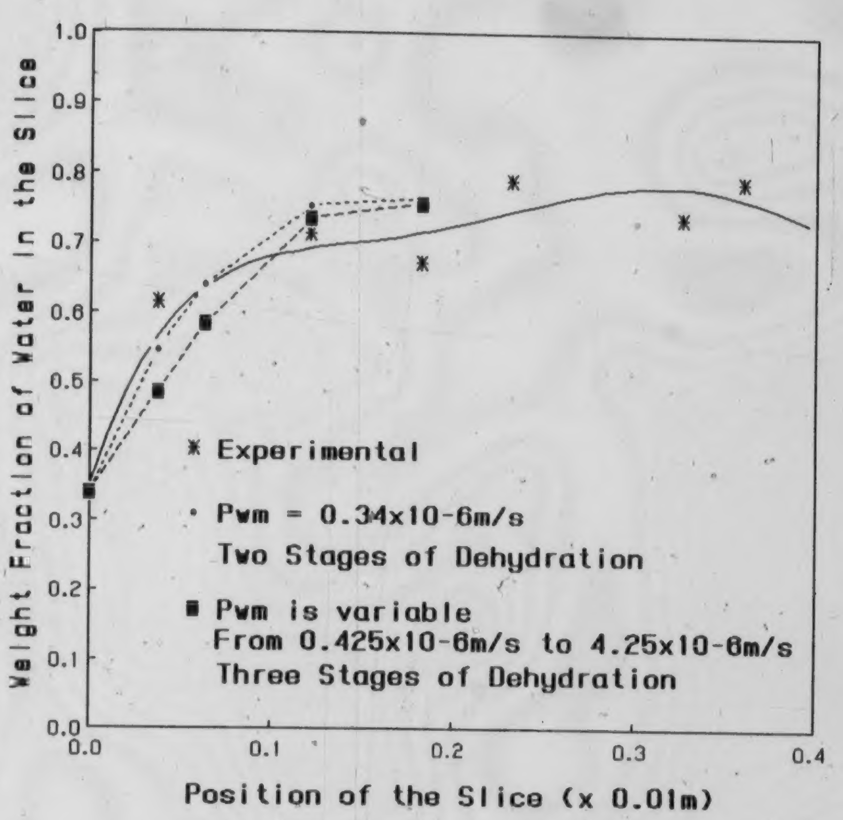

Fig. 4.7 Comparison between the Experimental and the Predicted Values of Moisture Content.

On fig. 4.6, it was found that the predicted profiles, that include the water transmembrane flux, match the experimental values of the weight fraction of sucrose in the tissue. Please note that the value of permeability coefficient was approximately 20 to 40 times smaller that the value reported in the literature by Rotstein and Cornish(1978b). The results seem to indicate a dependence of the permeability on the boundary layers on both sides of the plasmalemma which is particularly important at the surface where the sucrose concentration of the liquid phase of the extracellular space is 60%. This has been already indicated by Toupin(1986). Rotstein and Cornish(1978a) have also pointed out the importance of the boundary layers and the fact that the convective contribution to the water flux across membrane is often neglected in depicting the flux across membrane. Usually the permeability coefficients are measured in dilute solution. In that case, it is reasonable to expect that the permeability of water will be unaffected by the presence of other species. However, the sucrose concentration of sucrose in the extracellular space is particularly high at the surface and dilute at the centre. It can be expected that a resistance to the mass transfer at the surface of the membrane exists and affects the permeability coefficient. The lumped permeability would be smaller at the surface and greater at the centre affecting the profile accordingly. Rotstein and Cornish(1978a) have made a detailed analysis on the effect of the boundary layers on the permeability coefficients. Some simple considerations help to clarify the influence of the boundary layers and justify the use of permeability coefficients much lower than the literature value. If the cells are treated as isolated spheres, the classical heat/mass transfer expression for a single sphere of diameter d_c in a large body of motionless fluid can be used:

$$kc = \frac{2\bar{D}_s}{d_c} \qquad [4.107]$$

The value of the corrected diffusivity varies from $5.43\times10^{-10}m^2/s$ at infinite dilution to $1.08\times10^{-10}m^2/s$ for a 60% sucrose solution. Assuming that the diameter of the cell (d_c) is constant and equal to $1.80\times10^{-6}m$, the value of kc becomes $6.02\times10^{-6}m/s$ for the value of the diffusion coefficient at infinite dilution and $1.2\times10^{-6}m/s$ for the value of the diffusion coefficient corresponding to a 60% sucrose solution. Thus the effective permeability is calculated by:

$$\frac{1}{P_{wm}^{eff}} = \frac{1}{kc} + \frac{1}{P_{wm}} \qquad [4.108]$$

For kc = $6.02\times10^{-6}m/s$, $P_{wm}^{eff} = 4.25\times10^{-6}m^2/s$ and for kc = $1.2\times10^{-6}m^2s$, $P_{wm}^{eff} = 1.1\times10^{-6}m^2/s$. These values were used to carry out the simulations with a variable permeability coefficient.

Fig. 4.6 shows also that the penetration of sucrose into the tissue is increased considering that only a diffusion phenomenon takes place. The predicted sucrose concentration profile is overestimated in comparison with experimental values. There is no water coming out from the cellular volume through the plasmalemma to restrict the penetration of sucrose into the tissue.

Fig. 4.7 shows that the predicted values of water content are also in good agreement with the experimental values.

4.9.4 Sucrose and Water Fluxes at the Surface

Fig. 4.8 shows the values of the flux of sucrose at the surface as a function of the time of treatment. The z axis starts from zero at the centre. A negative value of the flux of sucrose reflects the net penetration of sucrose in the structure, whereas a positive value indicates that the sugar is being transported away from the surface. In the early stages of the osmotic treatment, a quick penetration of sucrose occurs in the first 100s. Sugar diffuses into the extracellular space of the structure enough to allow for an important difference in chemical potential between the extracellular space and the cellular volume so that a water flux coming from the cellular volume occurs through the plasmalemma. From 100s to 1800s of osmotic treatment, the sugar that has already penetrated in the tissue continues to diffuse. However, the flux of sugar at the surface being positive, the sugar is washed out by the water flux coming from the structure. As soon as the first cell reaches plasmolysis (around 2000s), the extracellular space opens up, sucrose penetrates more readily into the structure. This is also relected in the value of flux of sucrose at the surface which becomes negative again.

Fig. 4.9 represents the flux of water as a function of the time of osmosis. Water is lost from the structure at a constant rate and drops to a lower level as the cell reaches plasmolysis at around 1800s. At that time, the water removal at the surface seems limited by the sucrose that has penetrated the structure particularly when the surface area of

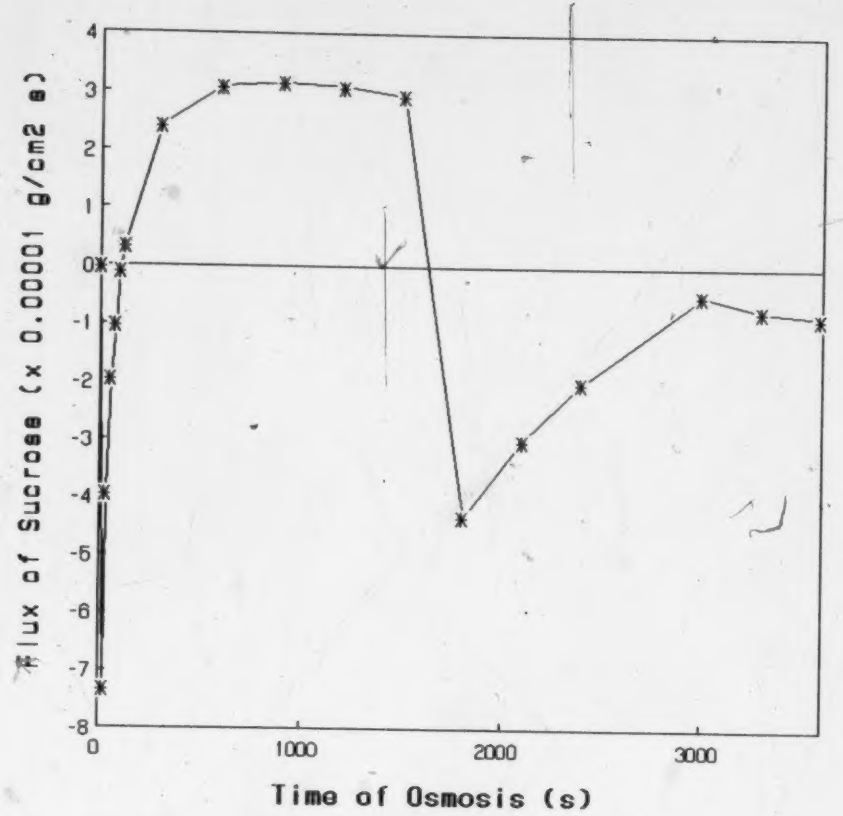

Fig. 4.8 Flux of Sucrose at the Surface
as Affected by the Time of Osmosis.

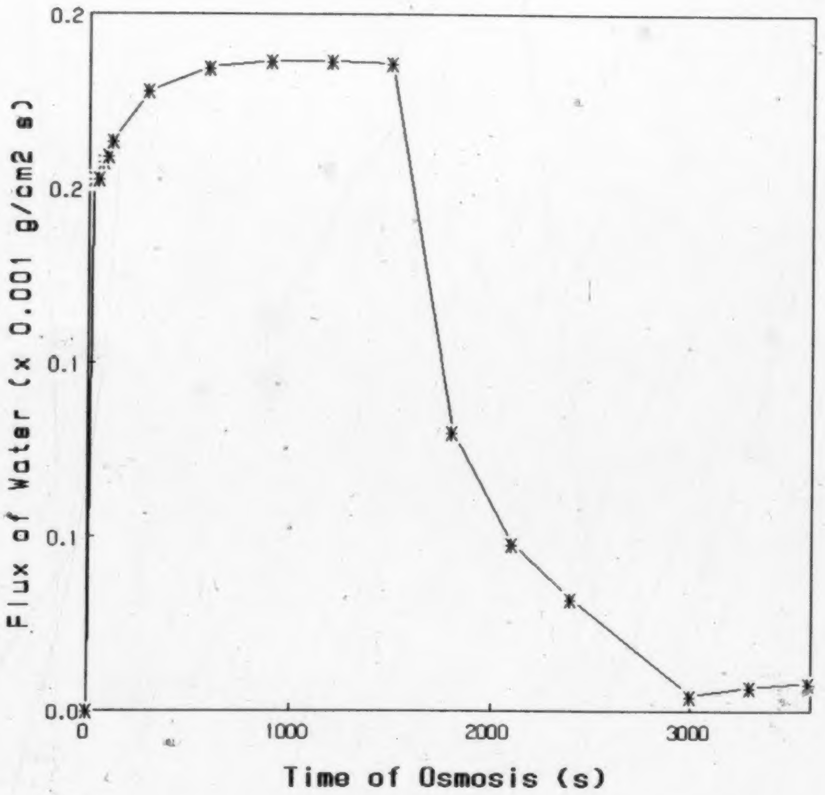

Fig. 4.9 Flux of Water at the Surface
as Affected by the Time of Osmosis.

the extracellular space increases. Lenart and Flink(1984b) have already pointed out the fact that for an osmotic treatment in a 60% sucrose solution the osmotic penetration depth is limited by the formation of the compacted surface layer with the result of a limited water removal.

Furthermore the model provides a powerful tool to monitor the changes that occur in the biological structure in order to understand the phenomena involved in the process as a function of time.

5. CONCLUSION AND RECOMMENDATIONS

In this study, the equilibrium experiment has shown that the extracellular space influences the behavior of potato tissue with respect to shrinkage.

A comparison between the calculated cell volumes from sorption data and the experimental cell volumes revealed that the calculated cell volumes match the experimental cellular volume for the whole range of sucrose solutions.

The vacuole of the cell was found to be mostly responsible for the loss of water in potato tissue particularly in the conditions of high water activity.

The equilibrium and the kinetic studies have also shown that not only the difference in chemical potential between the solution and the potato side but also the increase in the surface area of extracellular space influence the mass transport phenomena in potato tissue.

A geometrical equivalent of the potato cell has been used to develop a model which describes the mass transfer of sucrose in potato material (Toupin, 1986) with the main advantage of handling the diffusion in the extracellular space unidimensionally. Sorption properties of the potato tissue have been included for the thermodynamical description of the forces involved in the transmembrane flux.

Based on quantitative results, it is reasonable to conclude that the model proposed is able to describe the mass transport phenomena of potato tissue undergoing an osmotic treatment in a sucrose solution. This conclusion relies on the observed good agreement between the experimental and predicted data and on the fact that the simulations were carried out using microscopic properties of the tissue, which are relatively well documented in the literature, as well as using sorption properties. A comparison between experimental data of sucrose content and predicted values, considering a diffusion phenomenon only, indicates clearly that it is not possible to predict the results of sucrose content in biological structure after an osmotic treatment using the Fickian equation.

As pointed out by Toupin(1986) the most uncertain links in any analysis are the values given to the permeability coefficients of the membrane. From the results of the simulation it seems that the water permeability coefficient is dependent on the sucrose concentration of the extracellular space. It appears that boundary layers exist at the surface of the plasmalemma which affect the value of permeability coefficient. This study has revealed a general need for data on permeability coefficients.

Further studies are needed to investigate the influence of the turgor pressure on the cell behavior particularly at high values of water activity as well to estimate the elastic modulus of the wall and the general plasmolytic behavior of the plant cell for different fruits and vegetables.

The inclusion of the symplastic transport as a parameter of the model would have to be included although the proposed model represents quite well the behavior of the tissue structure.

Validation of the model should be done with other tissue structure.

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7. Appendix 1: Experimental Measurements and Data Calculations

7.1 Density Measurement

The densities were performed in the following manner:

1) The empty pycnometer was preweighed (m_{py}).
2) Potato material was added to the pycnometer and the pycnometer was weighed (m_{py+po}).
3) Distilled water at 23°C was added to the pycnometer and the pycnometer was reweighed ($m_{py+po+w}$).

Please note that prior to these measurements, the volume of the empty pycnometers were determined in the following manner:

1) Weigh the empty pycnometer (m_{py}).
2) Distilled water at 23°C was added and the pycnometer reweighed (m_{py+w}).
3) The steps 1 and 2 were repeated 5 times.

The densities (ρ) were calculated:

$$\rho = \frac{(m_{py+po} - m_{py})}{\left[\frac{(m_{py+w} - m_{py})}{\rho_{w,23^{\circ}C}}\right]^{*} - \left[\frac{(m_{py+po+w} - m_{py+po})}{\rho_{w,23^{\circ}C}}\right]} \qquad [7.1]$$

* Average of 5 measurements.

7.2 Total Solids Measurement

The total solids were performed in the following manner:

1) Weigh an empty aluminium dish (m_d).
2) Add some potato material in the dish and weigh the dish $(m_{d+po})_{before}$.
3) Dry in the air drying oven at 105oC for 24 hours and after cooling down in a dessicator under vacuum, weigh the dish $(m_{d+po})_{after}$.

The total solids (TS) were calculated:

$$TS = \frac{\left[[(m_{d+po})_{before} - m_d] - [(m_{d+po})_{after} - m_d]\right]}{[(m_{d+po})_{before} - m_d]} \times 100 \qquad [7.2]$$

7.3 Sugar Content Determination by HPLC

1) Some standard of sucrose, glucose, and fructose were run into the system to establish the standard curves. A linear regression was established between the peak height (PH) and the sucrose concentration (Y) of the standards.

$$Y = a\ (PH) + b \qquad [7.3]$$

The standard curves are plotted on fig. 7.1, fig. 7.2 and fig. 7.3 with their regression equation.

2) The unknown sample is then injected as an aliquot of the solution obtained from the extraction of the known weight of sample. The sucrose concentration (Y) is determined from the eq. [7.3] knowing the peak height (PH) obtained electronically by the Hewlett Packard integrator.

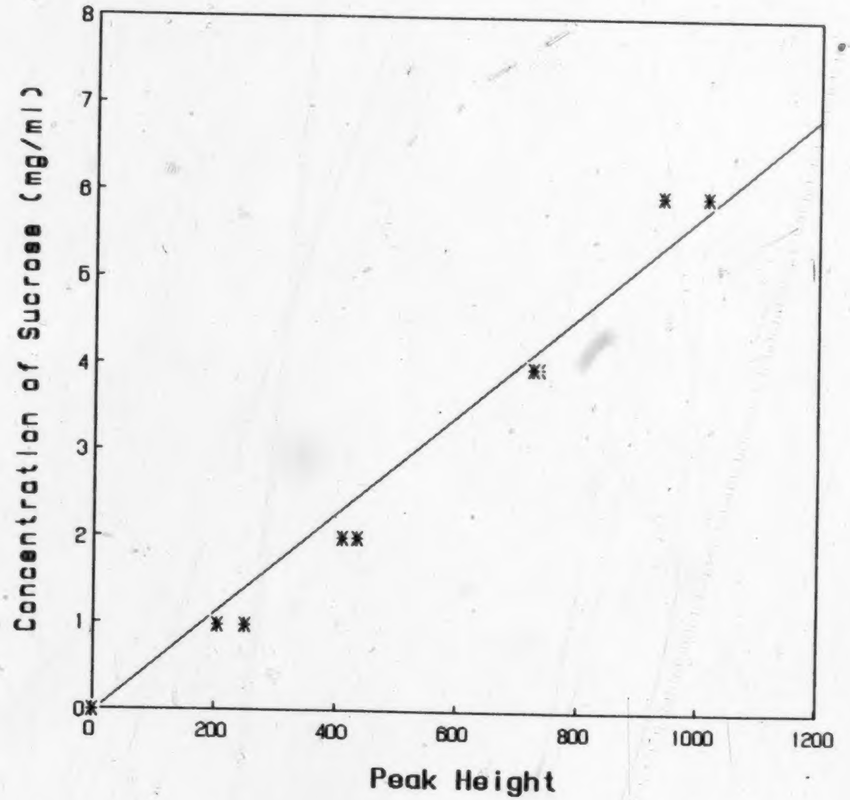

Fig. 7.1 Standard Curve for Sucrose.

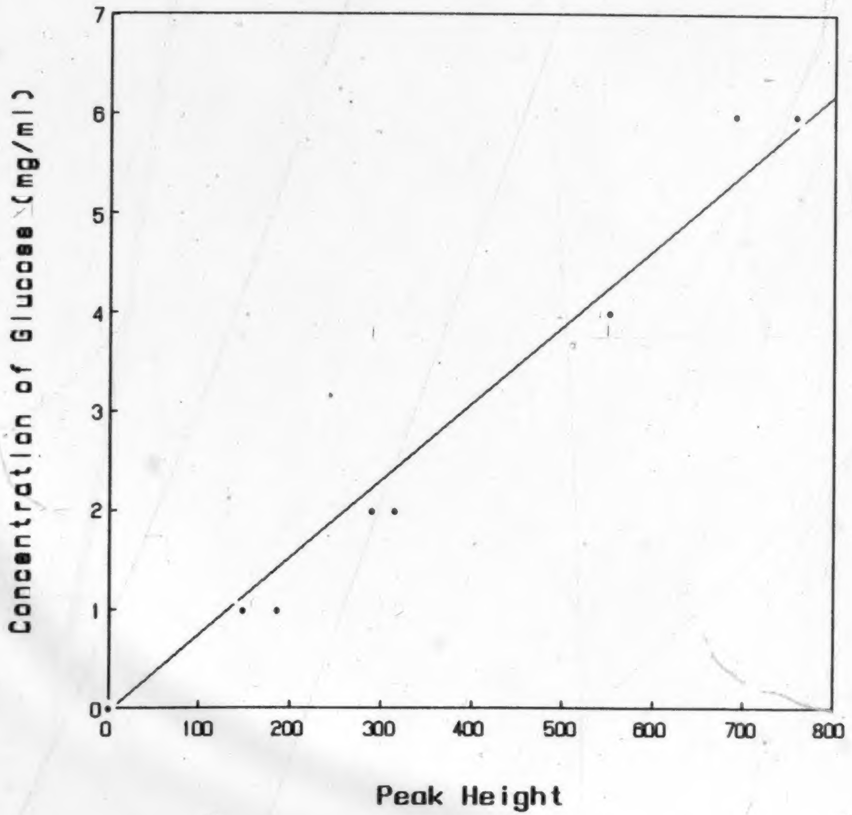

Fig. 7.2 Standard Curve for Glucose.

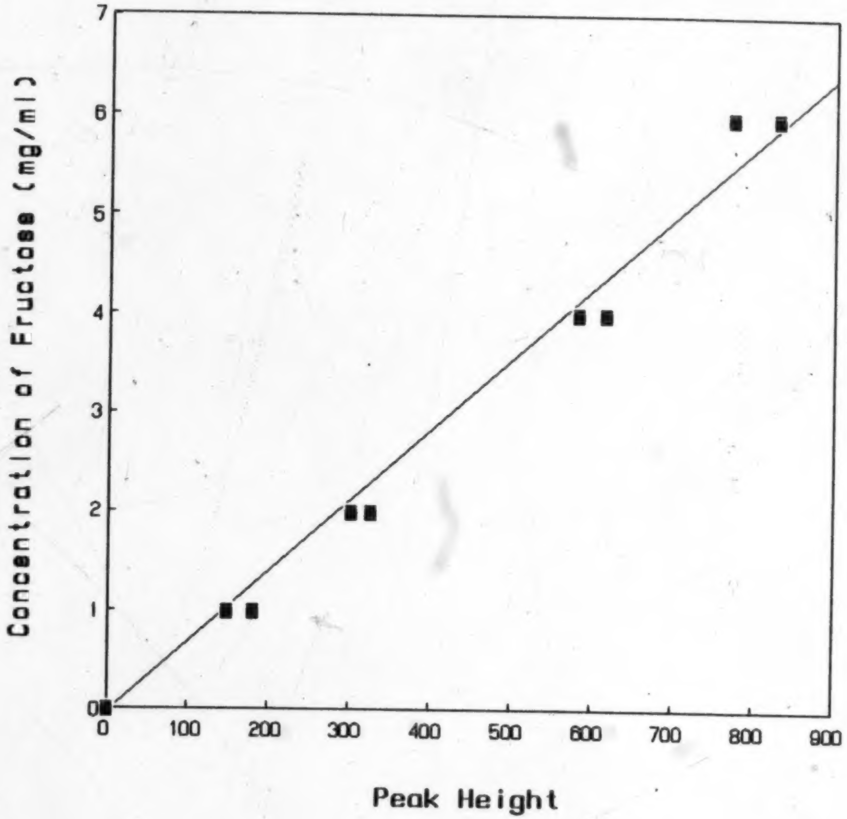

Fig. 7.3 Standard Curve for Fructose.

3) The sucrose content (SC) is calculated knowing the dilution factor (DF), or volume of the extraction solution, and the weight of potato sample (m_{po}):

$$SC = \frac{Y \times DF}{m_{po} \times 1000} \times 100 \qquad [7.4]$$

7.4 Insoluble Solids

The insoluble solids were calculated from the residue of the extraction.

1) An empty aluminium dish was preweighed (m_d).
2) The residue and the preweighed filter paper Whatman #4 (m_{filter}) were added to the dish.
3) After drying at 105°C for 24 hours in an air drying oven and cooling down in the dessicator under vacuum, the dish was reweighed $(m_{d+r})_{after}$.

Knowing the weight of potato sample, the insoluble solids (IS) are calculated in the following manner:

$$IS = \frac{\left[(m_{d+r})_{after} - m_d - m_{filter} \right]}{m_{po}} \times 100 \qquad [7.5]$$

7.5 Sugar Uptake Determination by the Isotope Dilution Method

1) Standards of ^{14}C were counted to establish the quench curve (fig. 7.4) which allows for the conversion of CPM to DPM measurement.

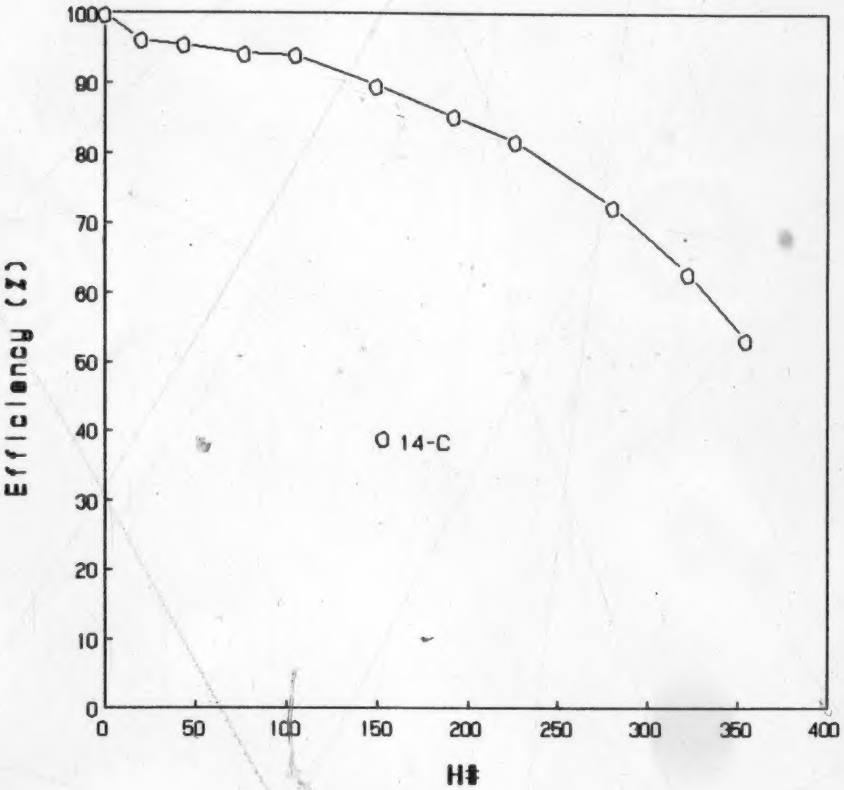

Fig. 7.4 Quench Curve for 14-C.

2) The mass of the sucrose solution (m_{sos}) as well as the volume of osmotic solution were recorded (V_{os}). A sample of the osmotic solution of known volume (V_{sa}) was counted (DPM_{os}).

3) Each osmosed slice was put in a preweighed vial (m_v) and weighed again (m_{v+po}).

4) The sample was digested or solubilized as described in section 3.2.2.4.2. of Material and Methods and counted (DPM_{po}).

The sugar uptake (SU) was determined:

$$SU = \frac{m_{sos} \times DPM_{po} \times V_{sa}}{DPM_{os} \times V_{os} \times (m_{v+po} - m_v)} \times 100 \qquad [7.6]$$

8. Appendix 2: Statistics on the Experimental Measurements of the Equilibrium Study

The statistics of the experimental measurements are shown in this appendix.

8.1 Density Measurements

8.1.1 Matrix of the Density Measurements

Blank 1	Fresh 2	5% 3	10% 4	20% 5	30% 6	40% 7	60% 8
1.0571	1.0722	1.087	1.1003	1.135	1.177	1.2101	1.3032
1.0473	1.1055	1.0947	1.0956	1.1507	1.1673	1.2047	1.3100
1.0691	1.1031	1.0523	0	1.1354	0	1.2197	1.3309
1.0569	1.0893	1.0693	1.0988	1.1235	1.1731	1.2108	1.3110
1.0646	1.0874	1.0713	1.0904	1.1259	1.1664	1.2174	1.3042
1.0563	1.0764	1.0783	0	1.1356	0	1.2033	1.3210
1.0579	0	1.0770	1.0955	1.1225	1.1723	1.2150	1.3103
0	0	1.1	1.1076	1.1265	1.1669	1.242	1.2994
0	0	1.0635	0	1.1335	0	1.1913	1.3180

where 0 indicates a missing data.

8.1.2 Anova table

	DF	SS	MS	F-RATIO
Treatment	7	0.42210	0.06030	512.349
Error	53	0.00624	0.00012	
Total	60	0.42833	-------	

Duncan Multiple Range Test Results

1 percent level: $1\ 3\ \underline{2\ 4}\ 5\ 6\ 7\ 8$

5 percent level: $1\ 3\ \underline{2\ 4}\ 5\ 6\ 7\ 8$

A line typed under any sequence of means indicates no significant difference at the given percent level.

8.2 Total Solids Measurements

8.2.1 Matrix of the Total Solids Measurements

Blank 1	Stored 2	5% 3	10% 4	20% 5	30% 6	40% 7	60% 8
14.71	21.37	21.35	26.64	34.5	39.04	46.26	64.69
17.90	22.19	22.02	24.51	31.00	39.18	45.05	64.62
13.93	22.95	21.85	0	31.84	0	45.16	66.03
14.96	21.13	18.41	25.75	32.98	41.18	45.44	66.15
13.90	18.80	15.12	24.52	30.36	39.14	45.90	65.93
14.74	19.74	23.37	0	33.21	0	45.50	65.73
15.15	19.20	14.57	28.54	33.74	38.92	47.03	64.41
14.10	22.25	22.82	26.36	31.63	39.84	46.51	65.10
0	20.80	0	0	32.53	0	45.14	65.51

where 0 indicates a missing data.

8.2.2 Anova table

	DF	SS	MS	F-RATIO
Treatment	7	16701.5085	2385.9298	893.6315
Error	56	149.5159	2.6699	-
Total	63	16851.0243	---------	

Duncan Multiple Range Test Results

1 percent level: 1 $\underline{3\ 2}$ 4 5 6 7 8

5 percent level: 1 $\underline{3\ 2}$ 4 5 6 7 8

A line typed under any sequence of means indicates no significant difference at the given percent level.

8.3 Mass Loss Measurements

8.3.1 Matrix of the Mass Loss Measurements

5% 1	10% 2	20% 3	30% 4	40% 5	60% 6
32.02	32.02	31.09	27.85	27.44	45.17
27.78	33.57	29.98	28.43	29.80	44.69
28.72	32.33	30.43	29.04	27.16	46.69

where 0 indicates a missing data.

8.3.2 Anova table

	DF	SS	MS	F-RATIO
Treatment	5	653.8592	130.7719	82.6789
Error	12	18.9802	1.5817	
Total	17	672.8394	-------	

Duncan Multiple Range Test Results

```
1 percent level:          5 4 1 3 2 6
                              -----
                          -------

5 percent level:          5 4 1 3 2 6
                                ---
                          -------
```

A line typed under any sequence of means indicates no significant difference at the given percent level.

The statistical analysis was performed using an APL program available on MTS(library 701 STP1; routine ANOVA2 and from FSTE:NEWSTAT, routine AN2DUNCGROUP).

9. Appendix 3: Error Propagation on the Experimental Equilibrium Parameters

The error analysis of the equilibrium calculated parameters such as the water loss (WL), the sugar gain (SG), the insoluble solids loss (ISL), the calculated total (V/V^{o}), the extracellular volume (V_i/V^{o}) and the cellular volume (V_c/V^{o}) shows that it is a function of few experimental measurements. Consequently, the error has to be propagated through. The relative error is used to calculate the error on the multiplication or the division of independent terms whereas the absolute error is used to calculate the error on a sum or a difference of independent terms.

9.1 Error Propagation on the Water Loss

Recalling that:

$$WL = \Big[\big[(1 + ML/100)\ (1 - TS/100)\big] - (1 - TS^{o}/100)\Big]\ 100 \qquad [9.1]$$

The relative error on the water loss measurement is calculated by:

$$\frac{\Delta WL}{WL} = \Bigg[(1 + ML/100)\ (1 - TS/100)\ \bigg[\frac{\Delta(1 + ML/100)}{(1 + ML/100)} + \frac{\Delta(1 - TS/100)}{(1 - TS/100)}\bigg] + \frac{\Delta(1 - TS^{o}/100)}{(1 - TS^{o}/100)}\Bigg]\ \Big[(1 + ML/100)\ (1 - TS/100) - (1 - TS^{o}/100)\Big]^{-1} \qquad [9.2]$$

9.2 Error Propagation on the Insoluble Solids Loss

Recalling that:

$$ISL = IS(1 + ML/100) - IS^{o} \qquad [9.3]$$

The error on the insoluble solids loss determination is determined by:

$$\frac{\Delta ISL}{ISL} = \left[\left[\frac{\Delta IS}{IS} + \frac{\Delta(1 + ML)}{(1 + ML)}\right](1 + ML/100)\ IS\right] - \Delta IS^{o} \qquad [9.4]$$

9.3 Error Propagation on the Sugar Gain

Recalling that:

$$SG = SC\left[1 + \frac{ML}{100}\right] \qquad [9.5]$$

The error on the sugar gain measurement becomes:

$$\frac{\Delta SG}{SG} = \frac{\Delta SC}{SC} + \frac{\Delta\left[\frac{ML}{100} + 1\right]}{\left[\frac{ML}{100} + 1\right]} \qquad [9.6]$$

9.4 Error Propagation on the Sugar Gain by Difference

Recalling that:

$$SGD = ((1 + ML/100)\ TS) - TS^{o} \qquad [9.7]$$

The relative error on the sugar gain by difference is calculated by:

$$\frac{\Delta SGD}{SGD} = \left[(1 + ML/100)\ TS \left[\frac{\Delta(1 + ML/100)}{(1 + ML/100)} + \frac{\Delta TS}{TS}\right] - \Delta TS^{o}\right]$$

$$/\ ((1 + ML/100)\ TS) - TS^{o} \qquad [9.8]$$

9.5 Error Propagation on the Experimental Total Volume, Extracellular Volume and Cellular Volume

Recalling that:

$$V/V^{o} = \frac{(1 + ML/100)}{\rho} \rho^{o} \qquad [9.9]$$

$$V_i/V^{o} = \frac{SC(1 + ML/100)}{\rho_{sol}/1000} \rho^{o} \qquad [9.10]$$

$$V_c/V^{o} = (V - V_i)/V^{o} \qquad [9.11]$$

The error on each volume is defined as:

$$\frac{\Delta V/V^{o}}{V/V^{o}} = \frac{\Delta(1 + ML/100)}{(1 + ML/100)} + \frac{\Delta\rho}{\rho} + \frac{\Delta\rho^{o}}{\rho^{o}} \qquad [9.12]$$

where $\Delta(1 + ML/100)$ is the standard deviation of the mass loss measurement, $\Delta\rho$ is the standard deviation of the density of the osmosed sample and $\Delta\rho^{o}$ is the standard deviation of the density of the material at full turgor.

$$\frac{\Delta V_i/V^o}{V_i/V^o} = \frac{\Delta SC}{SC} + \frac{\Delta(1 + ML/100)}{(1 + ML/100)} + \frac{\Delta\rho^o}{\rho^o} \qquad [9.13]$$

where ΔSC is the standard deviation of the measurement of sucrose content, Δ(1 + ML) is the standard deviation of the mass loss measurement and $\Delta\rho^o$ is the standard deviation of the full turgor material. We assume that the ρ_{sol} has a negligible contribution to the error.

$$\frac{\Delta V_c/V^o}{V_c/V^o} = \frac{\Delta V/V^o + \Delta V_i/V^o}{V/V^o - V_i/V^o} \qquad [9.14]$$

The relative error of each measurement is used to calculate the absolute error or equivalent standard deviation associated with each determination. The comparison between treatments is done using a duncan multiple range test. The error mean square is estimate from the mean of the standard deviation of the each treatment mean which has been previously calculated by propagating the error. This error mean is squared. An APL program available on MTS was used to compute the results of the comparison of means (library 701 STP1, routine AMEH.MCTEST) for WL, ISL, SGD, SGD, V/V^o, V_i/V^o, V_c/V^o.

10. Appendix 4: Correction of the Water Activity due to Temperature

In this section the derivation of equations relating activity, concentration and temperature for binary water-sucrose solutions is done. For the following equations the subscripts pertain to the components are defined as follow:

1 = water

2 = sucrose

The variation of the activity with temperature particularly for water is defined by:

$$\frac{\partial \ln a_1}{\partial T} = \frac{-\bar{L}_1}{RT^2} \qquad [10.1]$$

where a_1 : Water activity.

T : Temperature.

$\bar{L}_1$: Relative partial molar enthalpy.

R : Gas constant.

Klotz and Rosenberg (1974) have shown that:

$$\bar{L}_1 = -\int_{\bar{L}_2^{\circ}}^{\bar{L}_2} \frac{n_2}{n_1}\, d\bar{L}_2 \qquad [10.2]$$

$$\bar{L}_2 = \phi L_2 + n_2 \left[\frac{\partial \phi L_2}{\partial n_2}\right]_{n_1} \qquad [10.3]$$

Expressions for the apparent relative molal enthalpy (ϕL_2) of sucrose solutions are reported by Gucker et al. (1939) and Stroth and Schonert (1977) at 20°C, 25°C and 30°C (Lee, 1987):

$$\phi L_2 = 128.9 m_2 \qquad T = 20^\circ C \qquad [10.4]$$

$$\phi L_2 = 134.6 m_2 \qquad T = 25^\circ C \qquad [10.5]$$

$$\phi L_2 = 140.2 m_2 \qquad T = 30^\circ C \qquad [10.6]$$

Since;

$$m_2 = \frac{n_2}{n_1 M_1/1000} \qquad [10.7]$$

and,

$$\partial n_2 = n_1 M_1/1000 \ \partial m_2 \qquad [10.8]$$

$$\bar{L}_1 = \frac{-1}{55.51} \int_{\bar{L}_2^\circ}^{\bar{L}_2} m_2 d\bar{L}_2 \qquad [10.9]$$

$$\bar{L}_2 = \phi L_2 + m_2 \frac{\partial \phi L_2}{\partial m_2} \qquad [10.10]$$

Finally, knowing that at $m_2 = 0$ for $\bar{L}_2^\circ$:

$$\frac{\partial \bar{L}_1}{\partial T} = \frac{-1}{55.51} \int_0^{m_2} m_2 \frac{\partial \left[\frac{\partial \bar{L}_2}{\partial T} \right]}{\partial m_2} \partial m_2 \qquad [10.11]$$

Since $\bar{L}_2 = 257.8\ m_2$ at $T = 20^\circ C$; $\bar{L}_2 = 269.2 m_2$ at $25^\circ C$; $\bar{L}_2 = 280.4 m_2$ at $30^\circ C$, the variation of $\bar{L}_2$ with the temperature is estimated. A linear regression shows that:

$$\frac{\partial \bar{L}_2}{\partial T} = 2.24 m_2 \qquad [10.12]$$

with $r = 0.99999$

and,

$$\frac{\partial \bar{L}_1}{\partial T} = \frac{-1}{55.51} \int_0^{m_2} m_2 \frac{\partial (2.24 m_2)}{\partial m_2} \partial m_2 \qquad [10.13]$$

$$\frac{\partial \bar{L}_1}{\partial T} = -0.02016 m_2^2 \qquad [10.14]$$

The integration is performed to give:

$$\bar{L}_1 = -\ 0.02016 m_2^2 T \qquad [10.15]$$

Recalling that:

$$\frac{\partial \ln a_1}{\partial T} = -\frac{\bar{L}_1}{RT^2} = \frac{0.02016m_2^2}{RT} \qquad [10.16]$$

The separation of variables is done:

$$d\ln a_1 = \frac{0.02016m_2^2}{RT}\, dT \qquad [10.17]$$

Finally, integrating the equation, one obtains:

$$\ln \frac{a_1^T}{a_1^{To}} = \frac{0.02016m_2^2}{R} \ln \frac{T}{To} \qquad [10.18]$$

where m_2 is the molality of sucrose and T is the temperature in Kelvin. Since the experimental data for the relative molal enthalpy were expressed in cal/mole, the universal gas constant (R) is equal to 1.987cal/mole K. Finally for any correction of temperature:

$$\ln \frac{a_w^T}{a_w^{To}} = 0.010146\ m_2^2 \ln \frac{T}{To} \qquad [10.19]$$

N.B. Although experimental data are available only within the range of 20°C to 30°C, this correction equation is applied to correct the water activity outside the range e. g. the water activity obtained from the freezing point depression.

11. Appendix 5: Transformation of the Data of the Kinetic Study

The sucrose uptake of the slices, the density of the slices and the moisture content of the slices were determined although not with the same potato material. These measurements are related through the mass of the slices. In order to represent them with respect to the depth of penetration, some transformations have to be made. A curve is established which relates the position in the potato medium to the mass of the slice.

$$\frac{m_{po}}{A} = \bar{\rho}_{po}\, \Delta z_{po} \qquad [11.1]$$

where m_{po} is the mass of the slice, A is the surface area, Δz_{po} is the thickness of the slice and $\bar{\rho}_{po}$ is the average density. The thickness of the slice is defined as:

$$\frac{V_{po}}{A} = \Delta z_{po} \qquad [11.2]$$

A relation is developped from the density measureme

$$\sum_{i=1}^{s} \frac{m_{po}}{A}\; f \left[\sum_{i=1}^{s} \frac{V_{po}}{A} \right] \qquad [11.3]$$

These relations are found to be linear. Fig. 11.1, fig. 11.2 and fig. 11.3 show the relationship for an treatment in a 20% sucrose

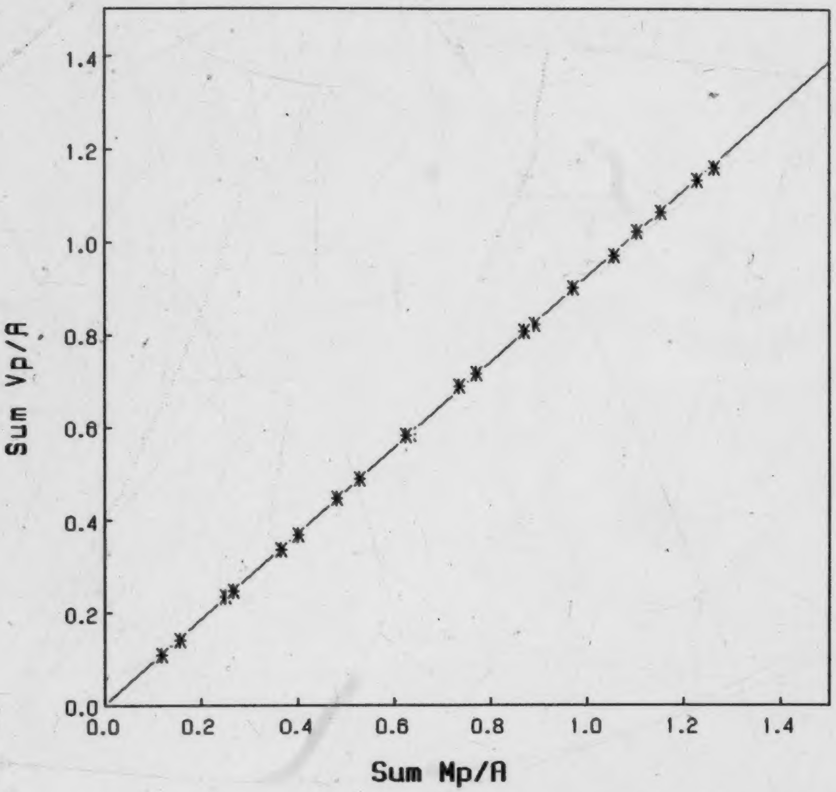

Fig. 11.1 Estimation of the Position of the Potato Slices from the Density Measurement for a 1 hour treatment in a 20% Sucrose Solution.

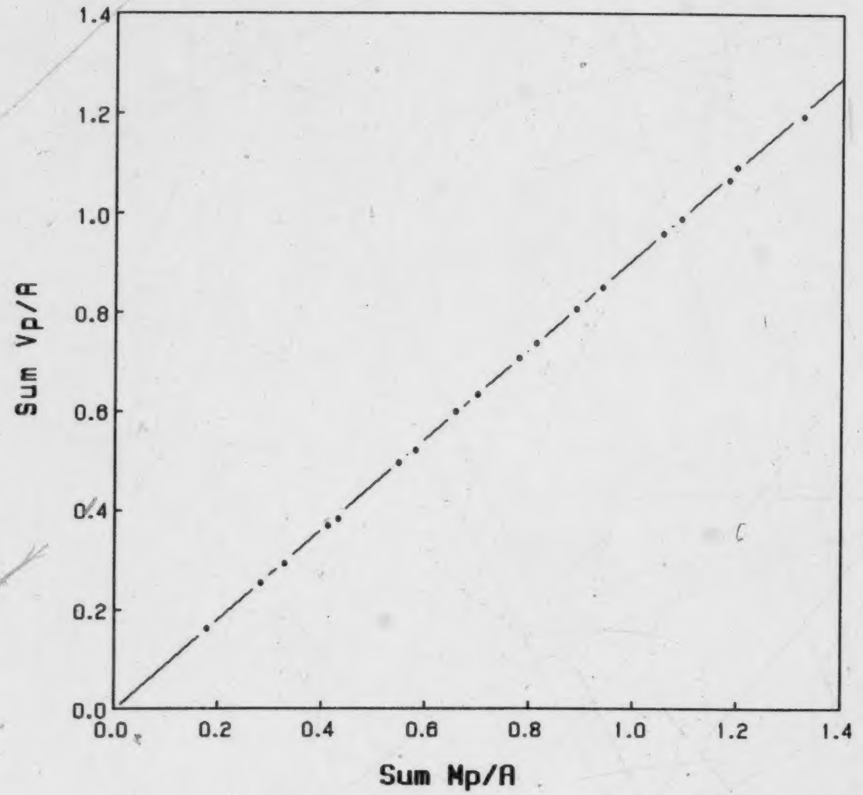

Fig. 11.2 Estimation of the Position of the Potato Slices from the Density Measurements for a 6 hour Treatment in a 20% Sucrose Solution.

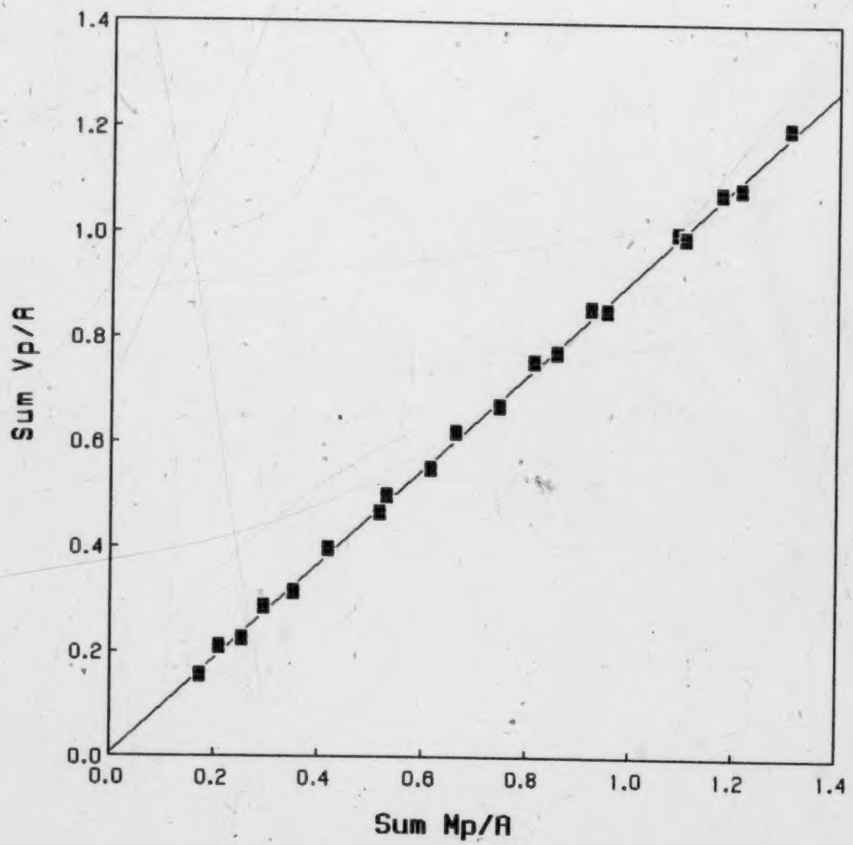

Fig. 11.3 Estimation of the Position of the Potato Slices from the Density Measurements for a 24 hour Treatment in a 20% Sucrose Solution.

solution for a time of 1 hour, 6 hours and 24 hours. Fig. 11.4, fig. 11.5 and fig. 11.6 represent the same relationship for an osmotic treatment in a 40% osmotic solution for a treatment of 1 hour, 6 hours and 24 hours. Finally, fig. 11.7, fig. 11.8 and fig. 11.9 show the relationship for an osmotic treatment in a 60% sucrose solution for a time of treatment of 1 hour, 6 hours and 24 hours.

In order to find the position attached to the measurements as a function of the depth of penetration. The values of $\sum \frac{m_{po}}{A}$ are calculated. The proper regression equation (i. e., representing the conditions of the sucrose concentration of the osmotic solution and the time duration of the treatment) is used to find the resulting position. The regression equations are listed in table 11.1 for each combination time of treatment and concentration of the osmotic solution. However, the position of the measurement has to be represented at half thickness of the potato slice. Please note that the data have been treated with Lotus 123.

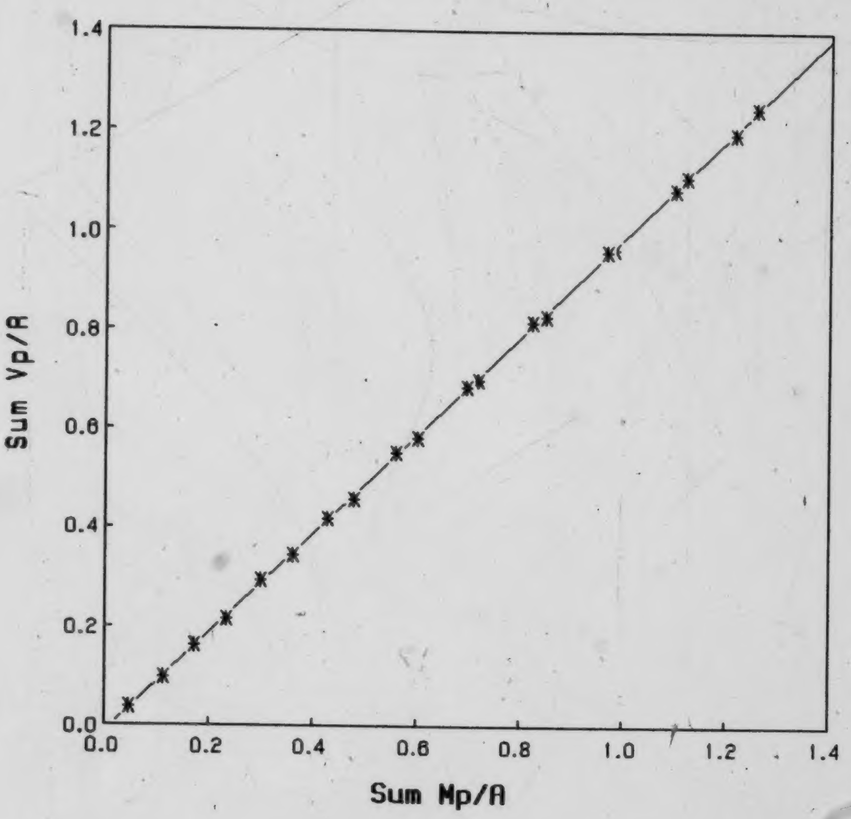

Fig. 11.4 Estimation of the Position of the Potato Slices from the Density Measurements for a 1 hour Treatment in a 40% Sucrose Solution.

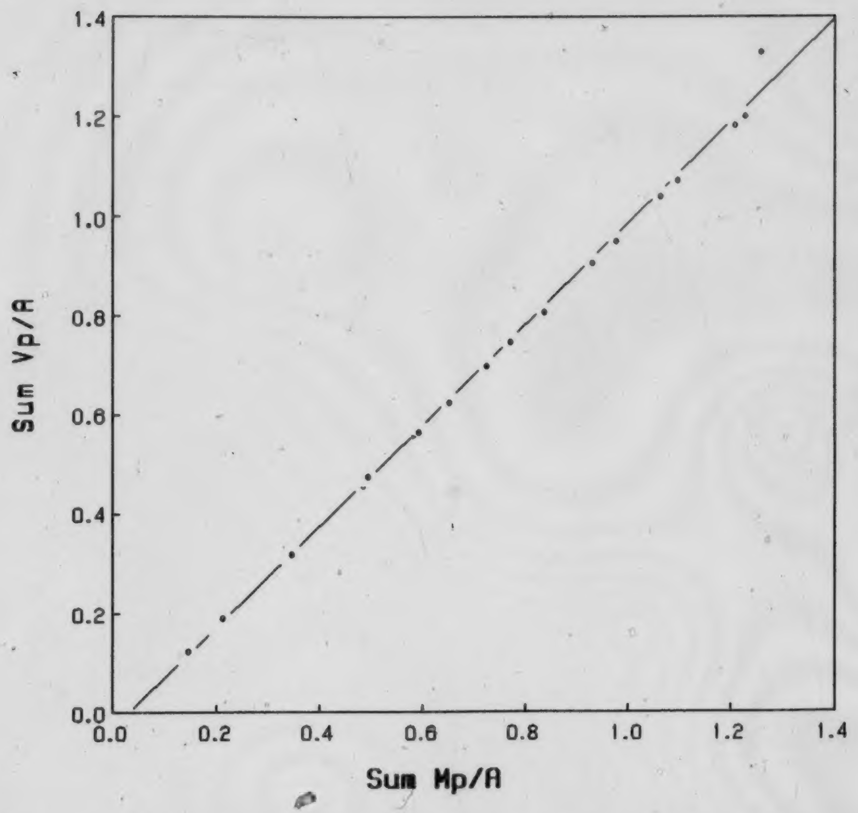

Fig. 11.5 Estimation of the Position of the Potato Slices from the Density Measurements for a 6 hour Treatment in a 40% Sucrose Solution.

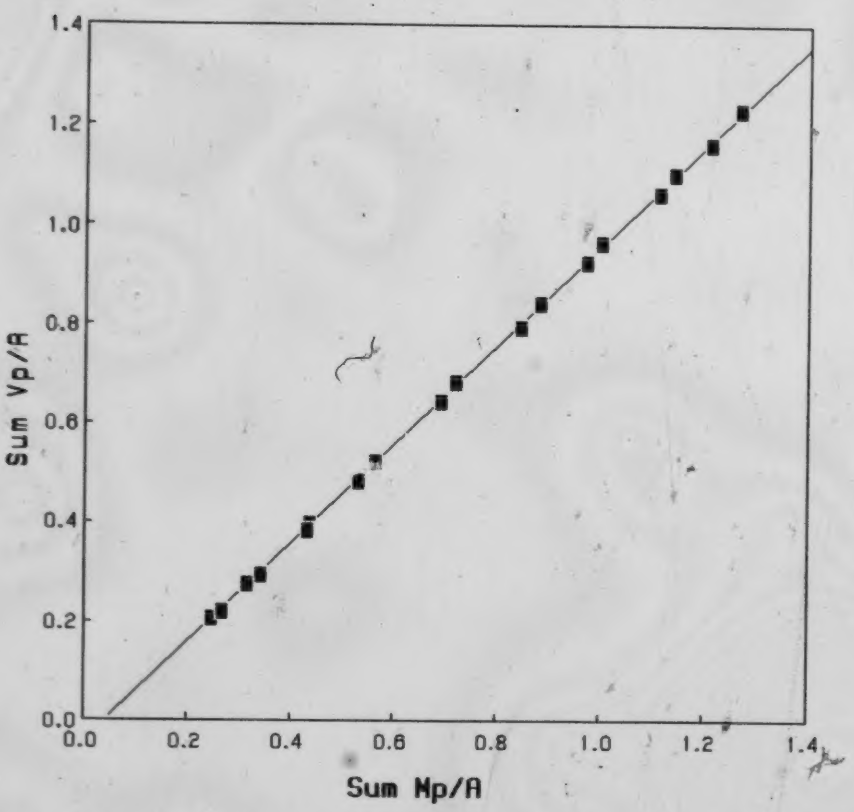

Fig. 11.6 Estimation of the Position of the Potato Slices from the Density Measurements for a 24 hour Treatment in a 40% Sucrose Solution.

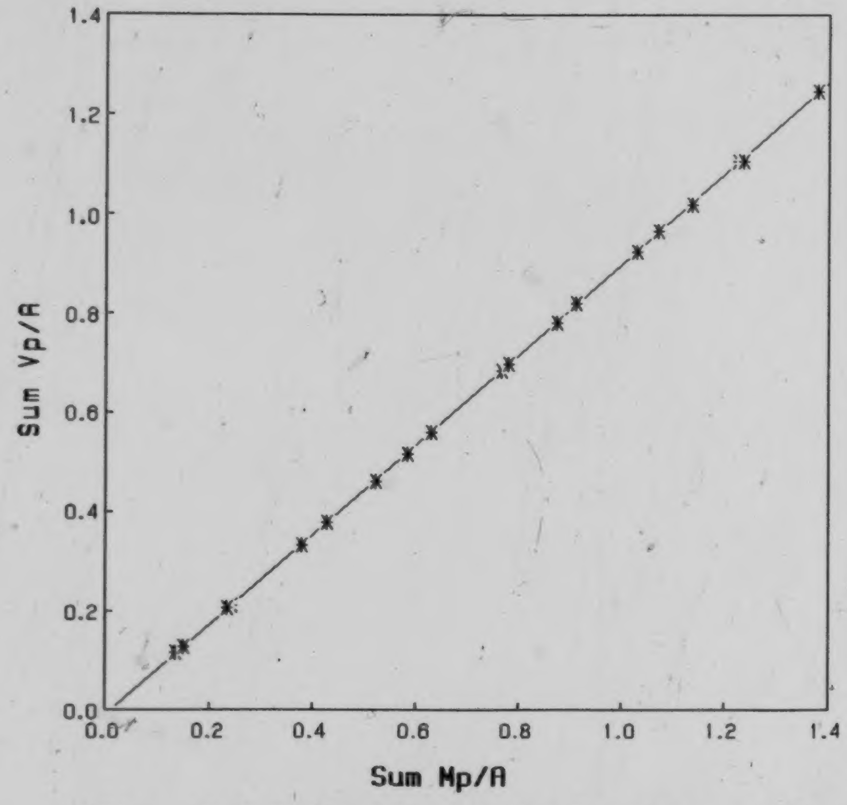

Fig. 11.7 Estimation of the Position of the Potato Slices from the Density Measurements for a 1 hour Treatment in a 60% Sucrose Solution.

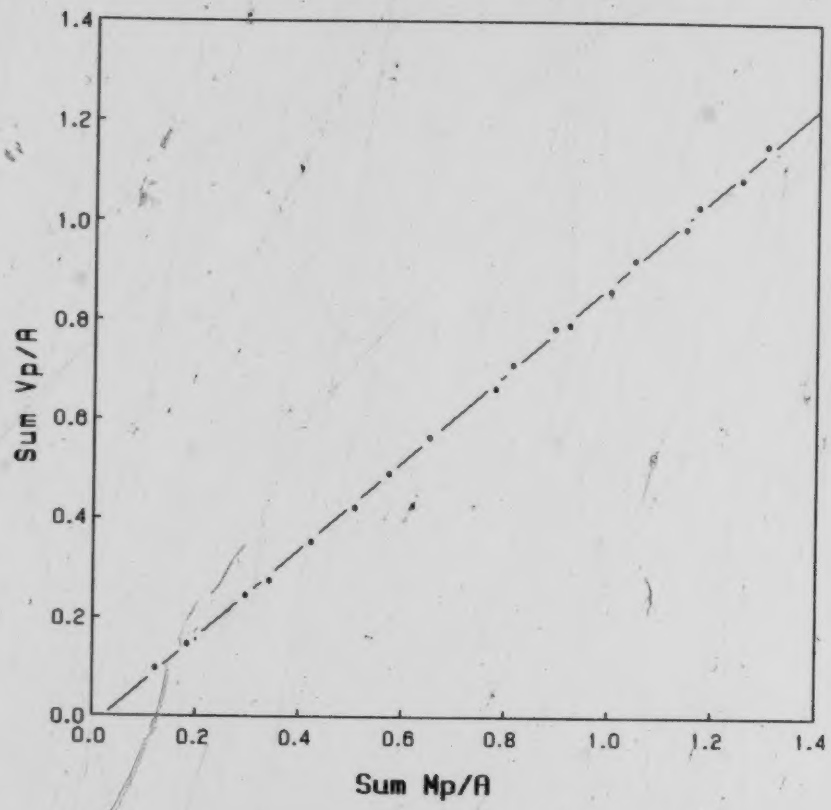

Fig. 11.8 Estimation of the Position of the Potato Slices from the Density Measurements for a 6 hour Treatment in a 60% Sucrose Solution.

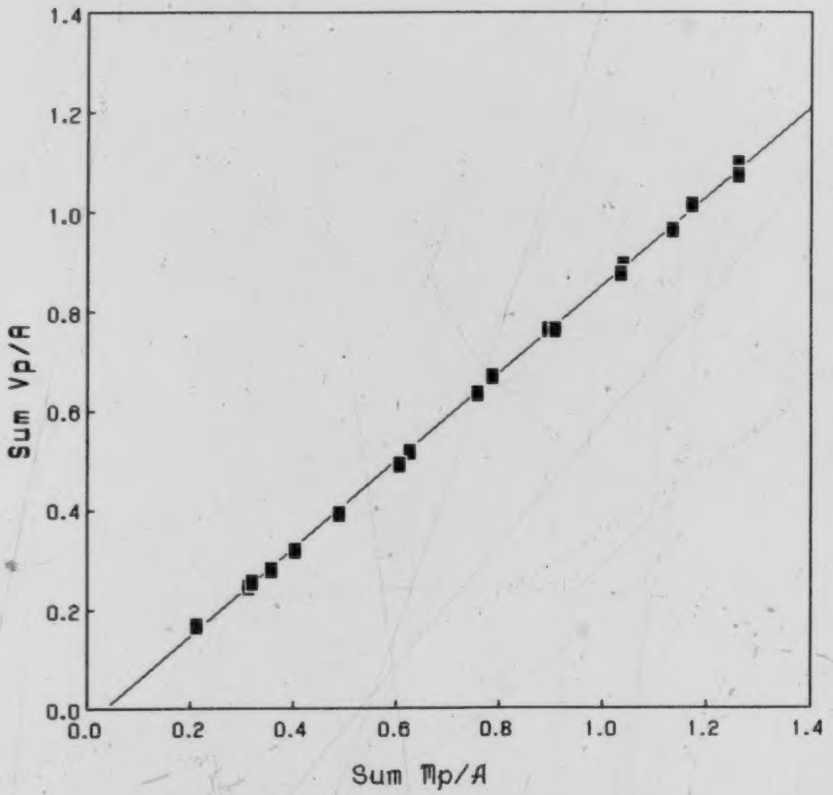

Fig. 11.9 Estimation of the Position of the Potato Slices from the Density Measurements for a 24 hour Treatment in a 60% Sucrose Solution.

Table 11.1 Regression Equations for the Position Correction.

Solution Concentration (%)	Time (hour)	Regression Equation
20	1	Y = 0.00127 + 0.9259 X
20	6	Y = -0.00298 + 0.9112 X
20	24	Y = 0.00660 + 0.9051 X
40	1	Y = -0.01173 + 0.9996 X
40	6	Y = -0.03269 + 1.0201 X
40	24	Y = -0.04317 + 1.0002 X
60	1	Y = -0.01072 + 0.9118 X
60	6	Y = -0.02038 + 0.8939 X
60	24	Y = -0.03154 + 0.8857 X

Y represents the value of Sum (Vp/A) and X represents the Sum (Mp/A)

12. Appendix 6: Changes of Volume upon Mixing Sucrose and Water

This section shows that the change of volume on mixing sucrose and water is negligible even with high concentrated sucrose solutions. Considering a 60% sucrose solution at 20°C, which is the maximum concentration of sucrose solution used experimentally, it can be found from the literature (Weast, 1984): $\rho_{mix}^{exp} = 1.2887 g/cm^3$, $\rho_s = 1.5805 g/cm^3$.

$$\frac{1}{\rho_{mix}^{exp}} = \bar{V}_{mix}^{exp} = 0.7760 cm^3/g \qquad [12.1]$$

$$\frac{1}{\rho_{mix}^{cal}} = \bar{V}_{mix}^{cal} = \frac{W_s}{\rho_s} + \frac{W_w}{\rho_w} = \frac{0.6}{1.5805} + \frac{0.4}{0.9982} = 0.7803 \qquad [12.2]$$

$$\bar{V}_{mix}^{cal} = 0.7803 cm^3/g$$

$$\%\ \text{Volume change due to mixing} = \frac{\bar{V}_{mix}^{cal} - \bar{V}_{mix}^{exp}}{\bar{V}_{mix}^{cal}} \times 100 = 0.56\% \qquad [12.3]$$

Consequently, the change of volume due to the mixing of sucrose and water is negligible.

13. Appendix 7: Diffusion Coefficients as affected by by the Frame of Reference.

The purpose of this appendix is to develop the diffusion coefficients based on the barycentric velocity using the method described by Yao(1981). The experimental measurements of diffusion coefficients are usually measured with respect to a fixed volume frame of reference i. e. volume average velocity. The mass average velocity is defined in case of a binary system sucrose water:

$$v = \omega_w v_w + \omega_s v_s \qquad [13.1]$$

and the volume average velocity:

$$v^{\circ} = \rho_w \frac{\bar{V}_w}{M_w} v_w + \rho_s \frac{\bar{V}_s}{M_s} \qquad [13.2]$$

The diffusional flux can be defined with respect to the mass average velocity and volume average velocity as follows:

$$J_i = \rho_i \left(v_i - v\right) \qquad [13.3]$$

$$J_i^{\circ} = \rho_i \left(v_i - v^{\circ}\right) \qquad [13.4]$$

where J_i is the diffusional flux with respect to the mass average velocity and J_i° is the diffusional flux with a fixed volume frame of reference.

It is important to point out that when dealing with diffusion problem J_i^o is commonly used which is the diffusional flux based on a volume frame of reference. The experimental diffusion coefficients are measured accordingly and named standard diffusion coefficients. In a binary system, only with a fixed volume frame of reference, there is an equality between the two diffusion coefficients. Consequently, a transformation between the experimental diffusion coefficients and the diffusion coefficients required by the model is needed since the equations developed involve the barycentric velocity instead of the volume average velocity. The conversion between fluxes is done. The diffusional flux can be divided in two parts as:

$$J_i = \rho_i (v_i - v^o) - \rho_i (v - v^o) \qquad [13.5]$$

Since $J_i^o = \rho_i (v_i - v^o)$, the diffusional flux based on the mass average velocity can be related to the diffusional flux based on the volume average velocity by the following equation:

$$J_i = J_i^o - \rho_i (v - v^o) \qquad [13.6]$$

Since $v = \Sigma \omega_k v_k$:

$$J_i = J_i^o - \rho_i (\Sigma \omega_k v_k - v^o) \qquad [13.7]$$

Multiplying the second term by ρ_k, dividing also by ρ_k and taking the summation out gives:

$$J_i = J_i^o - \rho_i \Sigma \frac{\omega_k}{\rho_k} \rho_k (v_k - v^o) \qquad [13.8]$$

and since $J^o_k = \rho_k \ (v_k - v^o)$

$$J_i = J^o_i - \rho_i \ \Sigma \ \frac{\omega_k}{\rho_k} \ J^o_k \qquad [13.9]$$

For our binary system:

$$J_w = J^o_w - \rho_w \left[\frac{\omega_w}{\rho_w} \ J^o_w + \frac{\omega_s}{\rho_s} \ J^o_s \right] \qquad [13.10]$$

$$J_s = J^o_s - \rho_s \left[\frac{\omega_w}{\rho_w} \ J^o_w + \frac{\omega_s}{\rho_s} \ J^o_s \right] \qquad [13.11]$$

Finally,

$$J_w = J^o_w \ (1 - \omega_w) - \frac{\omega_s \rho_w}{\rho_s} \ J^o_s \qquad [13.12]$$

$$J_s = J^o_s \ (1 - \omega_s) - \frac{\omega_w \rho_s}{\rho_w} \ J^o_w \qquad [13.13]$$

Using the property which shows that the sum of the relative fluxes is zero, the relation between the mass fluxes is defined:

$$\Sigma \ \bar{V}_i J^o_i = 0 \qquad [13.14]$$

J^o_s can be expressed as a function of J^o_w of vice-versa:

$$J_s^{\circ} = - \frac{J_w^{\circ} \bar{V}_w}{\bar{V}_s} \qquad [13.15]$$

and,

$$J_w^{\circ} = - \frac{J_s^{\circ} \bar{V}_s}{\bar{V}_w} \qquad [13.16]$$

$$J_w = J_w^{\circ} (1 - \omega_w) - \frac{\omega_s \rho_w}{\rho_s} \left[\frac{-J_w^{\circ} \bar{V}_w}{\bar{V}_s} \right] \qquad [13.17]$$

and,

$$J_s = J_s^{\circ} (1 - \omega_s) - \frac{\omega_w \rho_s}{\rho_w} \left[\frac{-J_s^{\circ} \bar{V}_w}{\bar{V}_s} \right] \qquad [13.18]$$

Grouping the terms together:

$$J_w = \left[(1 - \omega_w) - \frac{\omega_s \rho_w \bar{V}_w}{\rho_s \bar{V}_s} \right] J_w^{\circ} \qquad [13.19]$$

$$J_s = \left[(1 - \omega_s) - \frac{\omega_w \rho_s \bar{V}_s}{\rho_w \bar{V}_w} \right] J_s^{\circ} \qquad [13.20]$$

Since $J_w^{\circ} = - \mathrm{D} \frac{\partial \rho_w}{\partial z}$, $J_s^{\circ} = - \mathrm{D} \frac{\partial \rho_s}{\partial z}$ and $J_w = D_w \frac{\partial \rho_w}{\partial z}$, $J_s = D_s \frac{\partial \rho_s}{\partial z}$ D_s and D_w can be expressed as a function of D which is the standard diffusion coefficient based on a fixed volume frame of reference.

$$\mathcal{D}_w = \frac{\omega_s\rho_s\bar{V}_s + \omega_s\rho_w\bar{V}_w}{\rho_s\bar{V}_s} \qquad [13.21]$$

$$\mathcal{D}_s = \frac{\omega_w\rho_w\bar{V}_w + \omega_w\rho_s\bar{V}_s}{\rho_w\bar{V}_w} \qquad [13.22]$$

Since $\rho_s\bar{V}_s + \rho_w\bar{V}_w = 1$:

$$\mathcal{D}_w = \frac{\omega_s}{\rho_s\bar{V}_s}\,D \qquad [13.23]$$

and,

$$\mathcal{D}_s = \frac{\omega_w}{\rho_w\bar{V}_w}\,D \qquad [13.24]$$

and,

$$\mathcal{D}_w = \frac{D}{\rho\bar{V}_s} \qquad [13.25]$$

and,

$$\mathcal{D}_s = \frac{D}{\rho\bar{V}_w} \qquad [13.26]$$

Based on the experimental measurements of D either $\mathcal{D}_w$ or $\mathcal{D}_s$ is estimated and used in the model equations. $\bar{V}$ is equal to V/M.

14. Appendix 8: Description of the Numerical Method

The partial differential equation describing the transport of sucrose in the interstitial volume of the cj-th ECUC composing the hypothetical representative column is a highly non linear parabolic PED since the term D, ψ, v, $\frac{\partial v}{\partial z}$, $\frac{\partial A_i}{\partial \theta}$ and Rwm are implicitly functions of the interstitium concentration. The relation is integrated numerically in order to obtain the transient profile of concentration of the sucrose in the interstitium.

A discretization is made in both direction z, the distance variable and θ, the time variable. The region between the center of the tissue i. e. z = 0 and the surface is divided along the z- axis into increments with grid points being placed in the interstitium and more specifically on two boundaries and on each interface demarcating the cells composing the column in order to allow for the space increment to vary from cell-to-cell. The values of these steps (h_{cj}) are separated by equal space increments defined as:

$$h_{cj} = 1 / (\#grp - 1) \qquad [14.1]$$

where #grp is the number of grid points in the cell (assumed to be constant and identical for all the cells). Two space grids are necessary to describe the interstitium domain. The standard space grid consists of a certain number of increments from the center to the surface. The extended space grid is necessary to monitor the column behavior on a cell-to-cell basis due to the discontinuities created at the interface between cells. The extended space grid contains supplementary points at the interface such that the conditions there can be described with respect to both sides. Please note that the cells are numbered from surface to the center whereas the grids are numbered from the center to the surface. The Crank-Nicolson scheme was selected and adapted from Toupin(1986) to solve numerically the partial differential equation and ensure valid simulations. Recalling eq.[4.46]:

$$\frac{\partial \rho_s}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_s \frac{\partial \rho_s}{\partial z} \right] - v \frac{\partial \rho_s}{\partial z} - \rho_s \left[\frac{\partial v}{\partial z} + \frac{1}{A_i} \frac{\partial A_i}{\partial \theta} \right] \qquad [14.2]$$

In terms of central difference analog the first term or diffusional term on the RHS is defined as:

$$\frac{\partial}{\partial z}\left[\bar{D}_s \frac{\partial \rho_s}{\partial z} \right]_n^{j+1/2} = \frac{1}{h_{cj}^{j+1/2}} \left[\left[\frac{\bar{D}_{s\,n+1/2}^{\,j+1/2} \left[\rho_{s_{n+1}}^{j+1/2} - \rho_{s_n}^{j+1/2} \right]}{h_{cj}^{j+1/2}} \right] - \left[\frac{\bar{D}_{s\,n-1/2}^{\,j+1/2} \left[\rho_{s_n} - \rho_{s_{n-1}}^{j+1/2} \right]}{h_{cj}^{j+1/2}} \right] \right] \qquad [14.3]$$

The terms involving values estimated at the $j+1/2$ time level are approximated by arithmetic average of the finite difference analog.

$$\rho_{s_n}^{j+1/2} = 0.5 \left[\rho_{s_n}^{j+1} + \rho_{s_n}^{j} \right] \qquad [14.4]$$

Finally,

$$\frac{\partial}{\partial z}\left[\bar{D}_s \frac{\partial \rho_s}{\partial z}\right]_n^{j+1/2} = \frac{1}{2\left[h_{cj}^{j+1/2}\right]^2}\Bigg[\bar{D}_{s\;n+1/2}^{\;j+1/2}\;\rho_{s_{n+1}}^{j+1}$$

$$- \left[\bar{D}_{s\;n+1/2}^{\;j+1/2} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\right]\rho_{s_n}^{j+1} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\;\rho_{s_{n-1}}^{j+1} + \bar{D}_{s\;n+1/2}^{\;j+1/2}\;\rho_{s_{n+1}}^{j}$$

$$- \left[\bar{D}_{s\;n+1/2}^{\;j+1/2} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\right]\rho_{s_n}^{j} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\;\rho_{s_{n-1}}^{j}\Bigg] \qquad [14.5]$$

where:

$$\bar{D}_{s\;n+1/2}^{\;j+1/2} = f\left[0.5\left[\rho_{s_{n+1}}^{j+1/2} + \rho_{s_n}^{j+1/2}\right]\right] \qquad [14.6]$$

$$\bar{D}_{s\;n-1/2}^{\;j+1/2} = f\left[0.5\left[\rho_{s_n}^{j+1/2} + \rho_{s_{n-1/2}}^{j+1/2}\right]\right] \qquad [14.7]$$

Eq.[14.2] can be fully developped in terms of central difference analog to get:

$$\frac{\rho_{s_n}^{j+1} - \rho_{s_n}^{j}}{k^j} = \frac{1}{2\left[h_{cj}^{j+1/2}\right]^2}\Bigg[\bar{D}_{s\;n+1/2}^{\;j+1/2}\;\rho_{s_{n+1}}^{j+1}$$

$$-\left[\bar{D}_{s\;n+1/2}^{\;j+1/2} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\right]\rho_{s_n}^{j+1} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\,\rho_{s_{n-1}}^{j+1} + \bar{D}_{s\;n+1/2}^{\;j+1/2}\,\rho_{s_{n+1}}^{j}$$

$$-\left[\bar{D}_{s\;n+1/2}^{\;j+1/2} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\right]\rho_{s_n}^{j} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\,\rho_{s_{n-1}}^{j}\Bigg]$$

$$-\frac{1}{4h_{cj}^{j+1/2}}\left[v_n^{j+1/2}\left[\rho_{s_{n+1}}^{j+1} - \rho_{s_{n-1}}^{j+1}\right] + v_n^{j+1/2}\left[\rho_{s_{n+1}}^{j} - \rho_{s_{n-1}}^{j}\right]\right]$$

$$-\frac{1}{2}\Bigg[\left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^{j+1/2}\rho_{s_n}^{j+1}$$

$$+\left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^{j+1/2}\rho_{s_n}^{j}\Bigg] \qquad [14.8]$$

Regrouping all the terms involving values estimated at the advanced time level on the LHS leads to:

$$-\left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2}\bar{D}_{s\;n+1/2}^{\;j+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}}v_n^{j+1/2}\right]\rho_{s_{n+1}}^{j+1}$$

$$1 + \Bigg[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2}\left[\bar{D}_{s\;n+1/2}^{\;j+1/2} + \bar{D}_{s\;n-1/2}^{\;j+1/2}\right]$$

$$+ \frac{k^j}{2} \left[\left[\frac{\partial v}{\partial z} + \frac{1}{A_i} \frac{\partial A_i}{\partial \theta} \right]_n^{j+1/2} \right] \rho_{s_n}^{j+1}$$

$$- \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \bar{D}_{s\ n-1/2}^{\ j+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}} v_n^{j+1/2} \right] \rho_{s_{n-1}}^{j+1}$$

$$= \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \bar{D}_{s\ n+1/2}^{\ j+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}} v_n^{j+1/2} \right] \rho_{s_{n+1}}^{j}$$

$$1 - \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \left[\bar{D}_{s\ n+1/2}^{\ j+1/2} + \bar{D}_{s\ n-1/2}^{\ j+1/2} \right] \right.$$

$$\left. + \frac{k^j}{2} \left[\frac{\partial v}{\partial z} + \frac{1}{A_i} \frac{\partial A_i}{\partial \theta} \right]_n^{j+1/2} \right] \rho_{s_n}^{j}$$

$$+ \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \bar{D}_{s\ n-1/2}^{\ j+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}} v_n^{j+1/2} \right] \rho_{s_{n-1}}^{j} \qquad [14.9]$$

or,

$$- \mathrm{CMM1}_n^{j+1/2} \rho_{s_{n-1}}^{j+1} + (1 + \mathrm{CM}_n^{j+1/2}) \rho_{s_n}^{j+1} - \mathrm{CMP1}_n^{j+1/2} \rho_{s_{n+1}}^{j+1}$$

$$= \mathrm{CMM1}_n^{j+1/2}\ \rho_{s_{n-1}}^{j} + (1 - \mathrm{CM}_n^{j+1/2})\ \rho_{s_n}^{j} + \mathrm{CMP1}_n^{j+1/2}\ \rho_{s_{n+1}}^{j} \qquad [14.10]$$

At the surface:

$$\rho_s\big|_{s} = \rho_{sos} \qquad [14.11]$$

The analog becomes:

$$- \mathrm{CSM2}_{s-1}^{j+1/2}\ \rho_{s_{s-2}}^{j+1} + (1 + \mathrm{CSM1}_{s-1}^{j+1/2})\ \rho_{s_{s-1}}^{j+1}$$

$$= \mathrm{CSM2}_{s-1}^{j+1/2}\ \rho_{s_{s-2}}^{j} + (1 - \mathrm{CSM1}_{s-1}^{j+1/2})\ \rho_{s_{s-1}}^{j} + 2\mathrm{CB}_{s-1}^{j+1/2}\ \rho_{sos} \qquad [14.12]$$

where:

$$\mathrm{CSM2} = \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2}\ \bar{D}_{s\ \ s-1.5}^{\ \ j+1/2} + \frac{k^j}{4h_{cj}^{j+1/2}}\ v_{s-1}^{j+1/2} \right] \qquad [14.13]$$

$$\mathrm{CSM1} = \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \left[\bar{D}_{s\ \ s-0.5}^{\ \ j+1/2} + \bar{D}_{s\ \ s-1.5}^{\ \ j+1/2} \right] \right.$$

$$\left. + \frac{k^j}{2} \left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\ \frac{\partial A_i}{\partial \theta} \right]_{s-1}^{j+1/2} \right] \qquad [14.14]$$

$$CB = \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \bar{D}_{s\ s-0.5}^{\ j+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}} v_{s-1}^{j+1/2} \right] \qquad [14.15]$$

At the center:

$$\rho_s\big|_o = \rho_s^o \qquad [14.16]$$

The analog becomes:

$$(1 + C1)_1^{j+1/2}) \ \rho_{s_1}^{j+1} + C2_1^{j+1/2} \ \rho_{s_2}^{j+1}$$

$$= 2C0_1^{j+1/2} \ \rho_s^o + (1 - C1_1^{j+1/2}) \ \rho_{s_1}^j + C2_1^{j+1/2} \ \rho_{s_2}^j \qquad [14.17]$$

where:

$$C0 = \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \bar{D}_{s\ 0.5}^{\ j+1/2} + \frac{k^j}{4h_{cj}^{j+1/2}} v_1^{j+1/2} \right] \qquad [14.18]$$

$$C1 = \left[\frac{k^j}{2\left[h_{cj}^{j+1/2}\right]^2} \left[\bar{D}_{s\ 1.5}^{\ j+1/2} + \bar{D}_{s\ 0.5}^{\ j+1/2} \right] \right.$$

$$\left. + \frac{k^j}{2} \left[\frac{\partial v}{\partial z} + \frac{1}{A_i} \frac{\partial A_i}{\partial \theta} \right]_1^{j+1/2} \right] \qquad [14.19]$$

$$C2 = \left[\frac{k^{j}}{2\left[h_{cj}^{j+1/2}\right]^{2}} \bar{D}_{s\ 1.5}^{\ j+1/2} - \frac{k^{j}}{4h_{cj}^{j+1/2}} v_{1}^{j+1/2} \right] \qquad [14.20]$$

At the interface, at any time:

$$\left[A_i\ \bar{D}_s \frac{\partial \rho_s}{\partial z}\right]_{cj,in} = \left[A_i\ \bar{D}_s \frac{\partial \rho_s}{\partial z}\right]_{cj+1,in} \qquad [14.21]$$

"in" stands for interface. Recalling that the cell position index increases from surface to center while the grid point position index increases from center to surface, the forward analog is used for the derivative pertaining to the j-th cell and the backward for the j+1 derivative:

$$\left[\frac{\partial \rho_s}{\partial z}\right]_{cj,in}^{j+1/2} = \frac{1}{2\left[h_{cj}^{j+1/2}\right]} \left[\rho_{s_{cj,in+2}}^{j+1/2} + 4\rho_{s_{cj,in+1}}^{j+1/2} - 3\rho_{s_{cj,in}}^{j+1/2} \right] \qquad [14.22]$$

$$\left[\frac{\partial \rho_s}{\partial z}\right]_{cj,in}^{j+1/2} = \frac{1}{2\left[h_{cj}^{j+1/2}\right]} \left[\rho_{s_{cj,in-2}}^{j+1/2} + 4\rho_{s_{cj,in-1}}^{j+1/2} - 3\rho_{s_{cj,in}}^{j+1/2} \right] \qquad [14.23]$$

After inserting eq.[14.21] and eq.[14.22] into eq.[14.20],

$$- \rho_{s_{cj,in+2}}^{j+1/2} + 4\rho_{s_{cj,in+1}}^{j+1/2} - 3\rho_{s_{cj,in}}^{j+1/2}$$

$$= \phi^{j+1/2}_{cj+1} \left[\rho^{j+1/2}_{s_{cj+1}} - 4\rho^{j+1/2}_{s_{cj+1,in}} + 3\rho^{j+1/2}_{s_{cj+1,in}}\right] \qquad [14.24]$$

where:

$$\phi^{j+1/2}_{cj+1} = \left[\left[A_i\bar{D}_s\right]_{cj+1} h_{cj} \,/\, \left[A_i\bar{D}_s\right]_{cj} h_{cj+1}\right]^{j+1/2}_{in} \qquad [14.25]$$

The terms at the half time level are replaced by the arithmetic average of the analogs at the time levels j and j+1. After regrouping all the advanced time level terms on the LHS:

$$\begin{aligned}
&- \phi^{j+1/2}_{cj+1} \rho^{j+1}_{s_{cj+1,in-2}} + 4\phi^{j+1/2}_{cj+1,in} \rho^{j+1}_{s_{cj+1,in-1}} \\
&- (3 + 3\phi)^{j+1/2}_{cj+1,in} \rho^{j+1}_{s_{cj+1,in}} + 4\rho^{j+1}_{s_{cj,in+1}} - \rho^{j+1}_{s_{cj,in+2}} \\
&= \phi^{j+1/2}_{cj+1} \rho^{j}_{s_{cj+1,in-2}} - 4\phi^{j+1/2}_{cj+1,in} \rho^{j}_{s_{cj+1,in-1}} \\
&- (3 + 3\phi)^{j+1/2}_{cj+1,in} \rho^{j}_{s_{cj+1,in}} - 4\rho^{j}_{s_{cj,in+1}} + \rho^{j}_{s_{cj,in+2}} \qquad [14.26]
\end{aligned}$$

The mergence of the information pertaining to each of the two interface points into a unique quantity eliminates the need to use the extended space grid in the derivation. The set of linear equations leads to a matrix called a pentadiagonal band matrix which is solved using a method reported by Von Rosenberg(1969) and Toupin(1986).

The projection at half time level requires the analog at this level from the knowledge at j-th time level. Explicitly the value of $\rho_{s_n}^{j+1/2}$ is defined as:

$$\rho_{s_n}^{j+1/2} = \rho_{s_n}^{j} + \left[\frac{k^j}{2}\right] \frac{\partial \rho_{s_n}^{j}}{\partial \theta} \qquad [14.27]$$

The value of the derivative with respect to time is estimated by:

$$\frac{\partial \rho_{s_n}}{\partial \theta} = \frac{\partial}{\partial z}\left[\bar{D}_s \frac{\partial \rho_s}{\partial z}\right]_n^j - v_n^j \left[\frac{\partial \rho_s}{\partial z}\right]_n^j - \rho_{s_n}^j \left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^j \qquad [14.28]$$

From a finite difference analog point of view:

$$\frac{\partial \rho_{s_n}^j}{\partial \theta} = \frac{1}{\left[h_{cj}^j\right]^2}\left[\bar{D}_{s\ n+1/2}^{\ j}\ \rho_{s_{n+1}}^j - \left[\bar{D}_{s\ n+1/2}^{\ j} + \bar{D}_{s\ n-1/2}^{\ j}\right]\rho_{s_n}^j\right.$$

$$\left. + \bar{D}_{s\ n-1/2}^{\ j}\ \rho_{s_{n-1}}^j\right] - \frac{v_i^j}{2h_{cj}^j}\left[\rho_{s_{n+1}}^j - \rho_{s_{n-1}}^j\right]$$

$$- \rho_{s_n}^j \left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^{j+1/2} \qquad [14.29]$$

Finally,

$$\begin{aligned}\rho_{s_n}^{j+1/2} = \rho_{s_n}^{j} &+ \frac{k^j}{2\left[h_{cj}^{j}\right]^2}\left[\bar{D}_{s\ n+1/2}^{\ j} - \left[\bar{D}_{s\ n+1/2}^{\ j} + \bar{D}_{s\ n-1/2}^{\ j}\right]\right.\\ &\left. + \bar{D}_{s\ n-1/2}^{\ j}\right] - \frac{k^j}{4h_{cj}^{j+1/2}}\, v_n^j\left[\rho_{s_{n+1}} - \rho_{s_{n-1}}^{j}\right]\\ &+ \rho_{s_n}^{j}\,\frac{k^j}{2}\left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^j \qquad [14.30]\end{aligned}$$

Regrouping the terms:

$$\begin{aligned}\rho_{s_n}^{j+1/2} = &\left[\frac{k^j}{2\left[h_{cj}^{j}\right]^2}\,\bar{D}_{s\ n+1/2} - \frac{k^j}{4h_{cj}^{j+1/2}}\, v_n^j\right]\rho_{s_{n+1}}^{j}\\ &1 - \left[\frac{k^j}{2\left[h_{cj}^{j}\right]^2}\left[\bar{D}_{s\ n+1/2}^{\ j} + \bar{D}_{s\ n-1/2}^{\ j}\right]\right.\\ &\left. + \frac{k^j}{2}\left[\frac{\partial v}{\partial z} + \frac{1}{A_i}\frac{\partial A_i}{\partial \theta}\right]_n^j\right]\rho_{s_n}^{j}\\ &+ \left[\frac{k^j}{2\left[h_{cj}^{j}\right]^2}\,\bar{D}_{s\ n-1/2} + \frac{k^j}{4h_{cj}^{j}}\, v_n^j\right]\rho_{s_{n-1}}^{j} \qquad [14.31]\end{aligned}$$

Finally,

$$\rho_{s_n}^{j+1/2} = \mathrm{CMM1}_n^j \, \rho_{s_{n-1}}^j + (1 - \mathrm{CM}_n^j) \, \rho_{s_n}^j + \mathrm{CMP1}_n^j \, \rho_{s_{n+1}}^j \qquad [14.32]$$

Similarly, at the surface:

$$\rho_{s_{s-1}}^{j+1/2} = \mathrm{CSM2}_{s-1}^j \, \rho_{s_{s-2}}^j + (1 - \mathrm{CSM1}_{s-1}^j) \, \rho_{s_{s-1}}^j + \mathrm{CB}_{s-1}^j \, \rho_{sos} \qquad [14.33]$$

At the centre:

$$\rho_{s_1}^{j+1/2} = \mathrm{C0}_1^j \, \rho_s^o + (1 - \mathrm{C1}_1^j) \, \rho_{s_1}^j + \mathrm{C2}_1^j \, \rho_{s_2}^j \qquad [14.34]$$

At the interface between two cells:

$$- \rho_{s_{cj,in+2}}^{j+1/2} + 4\rho_{s_{cj,in+1}}^{j+1/2} - 3\rho_{s_{cj,in}}^{j+1/2}$$

$$= \phi_{cj+1}^{j+1/2} \left[\rho_{s_{cj+1}}^{j+1/2} - 4\rho_{s_{cj+1,in}}^{j+1/2} + 3\rho_{s_{cj+1,in}}^{j+1/2}\right] \qquad [14.35]$$

Since $\rho_{s_{cj,in}}^{j+1/2} = \rho_{s_{cj+1,in}}^{j+1/2}$;

$$\rho_{s_{cj+1,in}}^{j+1/2} = - \left[(3 + 3\phi)_{cj+1,in}^{j+1/2}\right]^{-1}$$

$$\left[\phi_{cj+1}^{j+1/2}\ \rho_{s_{cj+1,in-2}}^{j+1/2} - 4\phi_{cj+1,in}^{j+1/2}\ \rho_{s_{cj+1,in-1}}^{j+1\,2}\right.$$

$$\left.- 4\rho_{s_{cj,in+1}}^{j+1/2} + \rho_{s_{cj,in+2}}^{j+1/2}\right] \qquad [14.36]$$

15. Appendix 9: Calculation of the Water Activity: Program Listing

A computer program written in fortran 77 was developed to perform the numerical calculations of the complete composition of the potato cell (i. e., the water content of the starch, the water content of proteins, the water content of the vacuole) knowing the total water content and assuming that the phases are in equilibrium instantaneously (i. e., there is an equality of the water activity in the vacuole and the cytoplasm which comprises the starch and proteins) (Crapiste and Rotstein(1982).

A root finding subroutine (an IMSL subroutine, ZREAL2) was used to obtain the converge on the proper value of the water activity corresponding to the proper composition of each phase. Details are included in the program.

```
******************************************************************
*                        PROGRAM M.SORP                          *
******************************************************************
*                                                                *
* PURPOSE: THIS PROGRAM CALCULATES THE WATER CONTENT OF DIFFERENT *
*          PHASES OF THE POTATO CELLULAR VOLUME FROM A KNOWN      *
*          TOTAL WATER CONTENT USING A METHOD PROPOSED BY         *
*          CRAPISTE AND ROTSTEIN(1982).                           *
*                                                                *
* ON ENTRY                                                       *
*    WS,WG,WF - WEIGHT FRACTION OF SUCROSE, GLUCOSE, FRUCTOSE,    *
*     WKP,WKS   K3PO4, K2SO4, STARCH AND PROTEINS                 *
*      WST,WP   (MAIN COMPONENTS OF THE POTATO CELLULAR VOLUME    *
*               ON A DRY MATTER BASIS.                            *
*          XT - TOTAL WATER CONTENT OF THE CELLULAR VOLUME        *
*               ON A DRY MATTER BASIS.                            *
*                                                                *
* ON OUTPUT                                                      *
*         XST - WATER CONTENT OF THE STARCH                      *
*         XPR - WATER CONTENT OF PROTEINS                        *
*           X - WATER CONTENT OF THE VACUOLE                     *
*         PHI - WATER ACTIVITY OF THE CELLULAR VOLUME            *
*        PHIH - WATER ACTIVITY ESTIMATED BY HASLEY               *
*        PHIR - WATER ACTIVITY ESTIMATED BY RATTI                *
*                                                                *
*  EMPIRICAL CORRELATIONS ARE USED TO DETERMINE THE WATER        *
*  OF THE STARCH (XST) AND PROTEINS (XP). THEY WERE CORRELATED   *
*  BY CRAPISTE AND ROTSTEIN(1982).                               *
*                                                                *
*  FOR STARCH:                                                   *
*       RT LN PHI = RT LN (1 - EXP(-83.4768(XST**2.3015)))       *
*                                                                *
*  FOR PROTEINS:                                                 *
*       RT LN PHI = RT LN (-0.0206(XP**1.6128))                  *
*                                                                *
*  BY DIFFERENCE THE WATER CONTENT OF THE VACUOLE IS ESTIMATED   *
*  ON A BINARY BASIS, THE WATER ACTIVITY OF EACH COMPONENT OF    *
*  THE VACUOLE IS CALCULATED. USING THE ROSS(1975) EQUATION      *
*  THE WATER ACTIVITY OF THE VACUOLE IS ESTIMATED AND COMPARED   *
*  UNTIL CONVERGENCE ON THE PROPER VALUE WITH THE APPROPRIATE    *
*  COMPOSITION.                                                  *
******************************************************************

      INTEGER NSIG,N,ITMAX,IER
      REAL*8 MW,MG,MF,MS,MKP,MKS,B,C,R
      REAL*8 WG,WF,WS,WKP,WKS,WST,WP,F,EPS,EPS2,ETA,X
      REAL*8 ALG,ALF,ALS,ALKP,ALKS
      REAL*8 XST,XP,XT,PHI,T,PHIH
      REAL*8 C1,C2,C3,Q1,Q2,Q3,CX,QX,P0,PHIR,AWV
      COMMON/F1/WG,WF,WS,WKP,WKS,WP,WST,ALG,ALF,ALS,ALKP,ALKS,XT,
     &          XST,XP,X,AWV
      EXTERNAL F

* MOLECULAR WEIGHTS
*      WATER
         MW=18
*      GLUCOSE
         MG=180
*      FRUCTOSE
         MF=180
*      SUCROSE
         MS=342
*      K3PO4
         MKP=212
*      K2SO4
         MKS=174
*
* CONSTANTS FOR HASLEY EQUATION
      B=5.588D04
      C=1.048D0
      R=8314D0
      T=313.15

* CONSTANT FOR ROTSTEIN EQUATION
      C1=-2.87D-2
      C2=0
      C3=-1.858
      Q1=0.0107
      Q2=1.287
      Q3=-1.513
      P0=7.375

* CALCULATION OF ALP, CRAPISTE AND ROTSTEIN(1982)
      ALG=MW/MG
      ALF=MW/MF
      ALS=MW/MS
      ALKP=MW/MKP
      ALKS=MW/MKS

* READ THE DATA FOR THE COMPOSITION OF THE POTATO MATERIAL
      READ(1,*) WG,WF,WS,WKP,WKS,WST,WP

* READ THE TOTAL WATER CONTENT OF THE CELLULAR VOLUME
      READ(1,*) XT

* ESTIMATION OF FIRST GUESS ON THE WATER ACTIVITY BY THE
* HASLEY EQUATION
      PHI=DEXP(-B/(R*T*(XT**C)))

* CALL ZREAL2 SUBROUTINE TO COMPARE AWV AND PHI
* UNTIL CONVERGENCE. SETTING THE PARAMETERS USED IN ZREAL2
      EPS=1.0D-5
      EPS2=1.0D-3
      ETA=1.0D-3
      NSIG=5
      ITMAX=100
      N=1

*     CALL ZREAL2, AN IMSL SUBROUTINE TO FIND A ROOT.
      CALL ZREAL2(F,EPS,EPS2,ETA,NSIG,N,PHI,ITMAX,IER)

* ESTIMATION OF PHI WITH THE HASLEY CORRELATION.
      PHIH=DEXP(-B/(R*T*(XT**C)))

* CALCULATION OF PHI WITH THE RATTI CORRELATION.
      QX=Q1*DEXP(-Q2*XT)*(XT**Q3)
      CX=C1*DEXP(-C2*XT)*(XT**C3)
      PHIR=DEXP((QX*DLOG(P0))+CX)

* WRITING THE RESULTS
```

```
      WRITE(2,*)
      WRITE(2,1) 'SORPTION ISOTHERMS FOR POTATOES'
      WRITE(2,1) 'COMPOSITION'
      WRITE(2,1) 'VACUOLE'
      WRITE(2,2) 'WG= ',WG
      WRITE(2,2) 'WF= ',WF
      WRITE(2,2) 'WS= ',WS
      WRITE(2,2) 'WKP= ',WKP
      WRITE(2,2) 'WKS= ',WKS
      WRITE(2,1) 'CYTOPLASM'
      WRITE(2,2) 'WST= ',WST
      WRITE(2,2) 'WP= ',WP
      WRITE(2,*)
      WRITE(2,3) 'XV= ',X,'XST= ',XST,'XP= ',XP,'XT= ',XT
      WRITE(2,2) 'AWI= ',PHI
      WRITE(2,2) 'PHIN= ',PHIN
      WRITE(2,2) 'PHIR= ',PHIR
      WRITE(2,*)

  100 CONTINUE

    1 FORMAT(T16,A)
    2 FORMAT(T8,A,2X,F8.4)
    3 FORMAT(T8,A,F8.4,2X,A,F8.4,2X,A,F8.4,2X,A,F8.4)
    4 FORMAT(T8,A,F10.6,2X,A,F10.6)
      END

*****************************************************************
*                        SUBROUTINE F                           *
*****************************************************************
*                                                               *
* PURPOSE: THIS FUNCTION SUBROUTINE CALCULATES THE FUNCTION THAT  *
*          HAS TO BE OPTIMIZED. THE CONVERGENCE IS OBTAINED WHEN  *
*          WHEN TO CONSECUTIVE VALUES OF WATER ACTIVITY ARE EQUAL *
*          WITHIN A CERTAIN TOLERANCE. THIS FUNCTION SUBROUTINE   *
*          IS CALLED BY THE IMSL SUBROUTINE ZREAL2.               *
*****************************************************************

      REAL FUNCTION F(PHI)
      REAL*8 X
      REAL*8 XWG,XWF,XWS,XWKP,XWKS,WKP,WKS,WS,WG,WF,WP,WST
      REAL*8 ALG,ALF,ALS,ALKP,ALKS
      REAL*8 AWG,AWF,AWS,AWKP,AWKS,AWV,PHI
      REAL*8 XST,XP,XT
      COMMON/F1/WG,WF,WS,WKP,WKS,WP,WST,ALG,ALF,ALS,ALKP,ALKS,XT,
     &          XST,XP,X,AWV
*
* CALCULATION OF THE WEIGHT FRACTION OF WATER OF STARCH
* ON A DRY MATTER BASIS.
      XST=(-(DLOG(1-PHI))/53.4756)**(1/2.3015)
*
* CALCULATION OF THE WEIGHT FRACTION OF WATER OF PROTEINS
* ON A DRY MATTER BASIS.
      XP=(-(DLOG(PHI))/0.0208)**(-1/1.6129)
*
* CALCULATION OF THE WEIGHT FRACTION OF WATER OF THE VACUOLE
* ON A DRY MATTER BASIS BY DIFFERENCE.
      X=XT-(WST*XST)-(WP*XP)

* CALCULATION OF THE MOLE FRACTION OF EACH COMPONENT
* OF THE VACUOLE.
      XWG=X/(X+(WG*ALG))
      XWF=X/(X+(WF*ALF))
      XWS=X/(X+(WS*ALS))
      XWKP=X/(X+(WKP*ALKP))
      XWKS=X/(X+(WKS*ALKS))

* CALCULATION OF THE WATER ACTIVITY OF EACH COMPONENT
* OF THE VACUOLE ON A DRY MATTER BASIS.
      AWG=(10.**(-0.858*((1-XWG)**2.)))*XWG
      AWF=(10.**(-0.858*((1-XWF)**2.)))*XWF
      AWS=(10.**(-2.772*((1-XWS)**2.)))*XWS
      AWKP=(10.**(-0.718*((1-XWKP)**1.)))*XWKP
      AWKS=(10.**(-0.487*((1-XWKS)**1.)))*XWKS

* USING THE ROSS(1975) EQUATION THE WATER ACTIVITY OF THE
* VACUOLE IS CALCULATED.
      AWV=AWG*AWF*AWS*AWKP*AWKS

* THE WATER ACTIVITY OF THE VACUOLE IS COMPARED WITH THE VALUE
* OF THE TOTAL WATER ACTIVITY SINCE IT IS ASSUMED THAT THE
* WATER ACTIVITY OF THE VACUOLE IS EQUAL TO THE WATER ACTIVITY
* OF THE CYTOPLASM AND TO THE TOTAL WATER ACTIVITY.
      F=AWV-PHI

      RETURN
      END
```

16. Appendix 10: Theoretical Model: Program Listing

A computer program written in fortran 77 was developed to perform the numerical calculations of the theoretical model which attempted to describe the mass transport phenomena in potato tissue immersed in a sucrose solution.

A root finding subroutine (an IMSL subroutine, ZREAL2) was used to determine the complete composition of the cellular volume. A one dimensional quasi-cubic hermite interpolation procedure (an IMSL subroutine, IQHSCU) was used in conjunction with a cubic spline quadrature integration (an IMSL subroutine, DCSQDU) to compute the spline coefficients necessary to estimate the profile of the transmembrane fluxes and to carry the integration of those fluxes over the length of the cell under consideration. An interpolation procedure is used to compute point values of the concentration gradients through a cubic spline first derivative evaluator (an IMSL subroutine, DCSEVU). Details are included in the program m.tissue.for.

The program m.expcal is used in conjunction with m.tissue.for to evaluate the sucrose concentration, the water concentration and the density of the extracellular space and the cellular volume on a cell basis in order to compare the theoretical and experimental profiles for a given time.

A quasi-cubic hermite interpolation procedure (an IMSL subroutine, IQHSCU) was used in conjunction with a cubic spline quadrature integration (an IMSL subroutine, DSCQDU) to compute the spline coefficients necessary to estimate the profile of the sucrose concentration in the extracellular space and to carry out the integration over the entire length of the cell under consideration.

```
**********************************************************************
*
*   PROGRAM NAME   - M.TISSUE.FOR
*   LATEST VERSION  - JUNE 1988
*
*   PROGRAM TISSUE -  MODIFIED BY MICHELE MARCOTTE
*                       FOOD ENGINEERING GROUP
*                       DEPARTMENT OF FOOD SCIENCE
*                       UNIVERSITY OF ALBERTA
*                       EDMONTON, ALBERTA.
*
*   PURPOSE   - THIS PROGRAM SIMULATES THE ISOTHERMAL MASS TRANSPORT
*               PHENOMENA OCCURRING IN POTATO TISSUE IMMERSED IN A
*               SUCROSE SOLUTION.
*
*   REMARKS   - THE GEOMETRY IS SUCH THAT IT CAN BE ASSIMILATED TO
*               A SEMI-INFINITE MEDIUM.  AN EQUIVALENT CYLINDRICAL
*               CELL IS USED TO MODEL AS CLOSE AS POSSIBLE THE
*               AVERAGE PROPERTIES AND CHARACTERISTICS OF THE REAL
*               PLANT TISSUE.  BULK UNIDIRECTIONAL MASS TRANSFER
*               ONLY IS CONSIDERED.  IT IS ASSUMED THAT THE TISSUE
*               IS MACROSCOPICALLY HOMOGENEOUS AND ISOTROPIC.
*               THE REAL TISSUE IS ASSIMILATED TO A BUNDLE OF
*               COLUMNS MADE OF LINEAR ARRANGEMENTS OF UNIT
*               CYLINDRICAL CELLS. SINCE EACH COLUMN IS ASSUMED TO
*               BEHAVE IN A SIMILAR FASHION, ONLY ONE COLUMN IS
*               CONSIDERED FOR SIMULATION PURPOSE.
*
*               THE MODEL HAS BEEN DESIGNED TO ALLOW NOT ONLY FOR
*               APOPLASTIC TRANSPORT BUT ALSO FOR SYMPLASTIC
*               TRANSPORT.
*
*               IT IS ASSUMED THAT BOTH TYPES ARE OF A PASSIVE
*               NATURE. IT ALSO SIMULATES THE INTERNAL VARIATIONS
*               OF INTRA AND EXTRACELLULAR VOLUMES. IT ALLOWS FOR
*               POSSIBLE SHRINKAGE OF THE WHOLE STRUCTURE.
*
*   THE FOLLOWING CONSTANTS DETERMINE THE SIZE OF THE
*   ARRAYS TO BE USED IN THE PROGRAM.
*
*             NGRPTS - NUMBER OF GRID POINTS ON THE EXTENDED SPACE
*                      GRID ASSUMING A MAXIMUM OF 10 GRID POINTS
*                      PER UNIT CYLINDRICAL CELL TO BE MODELLED.
*                      MINIMUM NUMBER OF GRID POINTS IS 7 PER CELL.
*             NCELLS - MAXIMUM NUMBER OF UNIT CYLINDRICAL CELLS
*                      PRESENT IN THE MODEL COLUMN.
*
*   MAIN VARIABLES
*
*             NLEVEL - CURRENT TIME LEVEL, IN SEC.
*              TTIME - CURRENT TIME, IN SEC.
*                TIM - INTERNAL CLOCK (MILLISECONDS)
*              TSTEP - CURRENT INTEGRATION TIME STEP, IN SEC.
*              KSTEP - CURRENT INTEGRATION TIME STEP, IN SEC.
*             LVLCNT - TIME LEVEL COUNTER WHICH INDICATES THE TIME
*                      LEVEL CORRESPONDING TO THE DATA TO BE USED
*                      IN THE CALCULATIONS.
*               PCNT - COUNT OF OUTPUTS PERFORMED.
*              PTEST - TEST TO DETERMINE IF OUTPUT IS DESIRED OR
*                      NOT.
*             ITECNT - ITERATION COUNTER FOR CRANK-NICOLSON
*                      INTEGRATION ALGORITHM.
*                 TM - FLAG TO INDICATE IF THE VARIABLES HAVE TO BE
*                      FROM A FILE OR INITIALIZE FROM ZERO.
*               PINT - FLAG TO INDICATE IF INTERMEDIATE PROFILES
*                      ARE EXPECTED TO BE PRINTED.
*              PPINT - TIME AT WHICH INTERMEDIATE PROFILES
*                      ARE PRINTED.
*             STAGEV - VECTOR OF FLAGS INDICATING THE DEHYDRATION
*                      STAGE REACHED BY EACH UNIT CELL IN THE MODEL
*                      COLUMN. IF SET TO 1, THE CELL IS STILL IN
*                      TURGOR. IF SET TO 2, THE CELL IS PLASMOLYSED
*               CSIM - MATRIX OF INTERSTITIUM SUCROSE
*                      CONCENTRATIONS, IN G CM-3.
*               CSCM - MATRIX OF WATER CONCENTRATIONS, IN G WATER
*                      PER G DRY MATTER.
*                      CSCM(1, NCELLS, LVLCNT) = XT
*                      CSCM(2, NCELLS, LVLCNT) = XST
*                      CSCM(3, NCELLS, LVLCNT) = XP
*                      CSCM(4, NCELLS, LVLCNT) = XV
*              CELLM - MATRIX OF CELL MENSURATIONS.
*                      CELLM(1, NCELLS, LVLCNT) = VC
*                      CELLM(2, NCELLS, LVLCNT) = VI
*                      CELLM(3, NCELLS, LVLCNT) = VT
*                      CELLM(4, NCELLS, LVLCNT) = RC
*                      CELLM(5, NCELLS, LVLCNT) = RI
*                      CELLM(6, NCELLS, LVLCNT) = RB
*                      CELLM(7, NCELLS, LVLCNT) = LC
*                      CELLM(8, NCELLS, LVLCNT) = AI
*                      CELLM(9, NCELLS, LVLCNT) = IRESF
*
*              THE ABOVE MATRICES CONTAIN DATA CORRESPONDING TO 3
*              TIME LEVELS: N, N + 1/2 AND N + 1.
*
*             FLUXMM - VECTOR OF TRANSMEMBRANE FLUXES, IN G/CM2 SEC.
*             FLUXPM - MATRIX OF PLASMODESMAL FLUXES, IN G/CM2 SEC.
*               PDTM - VECTOR OF WATER PRODUCTION-DEPLETION
*                      IN G/CM2 SEC.
*              CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES,
*                      IN CM3/SEC.
*                      CVTDM(1, NCELLS) = DVC/DT
*                      CVTDM(2, NCELLS) = DVI/DT
*                      CVTDM(3, NCELLS) = DVT/DT
*              GPTDM - MATRIX OF GEOMETRICAL RELATION TIME
*                      DERIVATIVES.
*                      GPTDM(1, NCELLS) = DLC/DT
*                      GPTDM(2, NCELLS) = DRI/DT
*                      GPTDM(3, NCELLS) = DRC/DT
*                      GPTDM(4, NCELLS) = DRB/DT
*                      GPTDM(5, NCELLS) = DIRESF/DT
*                      GPTDM(6, NCELLS) = DAI/DT
*             VELGRV - VECTOR OF MASS AVERAGE VELOCITY GRADIENTS.
*               VELV - VECTOR OF MASS AVERAGE VELOCITIES, IN CM/SEC.
*             FLUXAM - MATRIX OF APOPLASTIC FLUXES G/CM2 SEC.
*                    COEFFICIENTS OF THE FINITE DIFFERENCE       *
*                    EQUATIONS (SEE SUBROUTINE NLCOEF FOR        *
*                    DETAILS, DIMENSIONLESS).                    *
*           OLDCIM - MATRIX CONTAINING ESTIMATES OF              *
*                    INTERSTITIUM CONCENTRATIONS AT THE N+1 TIME *
*                    LEVEL.                                      *
*            CTEST - TEST VALUE USED TO CHECK CONVERGENCE IN     *
*                    CRANK-NICOLSON INTEGRATION ALGORITHM.       *
******************************************************************

      PROGRAM TISSUE

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C6/ MWV(3)
      COMMON /C8/ GRTOL, GRSTEP, CNTOL, ITEMAX
      COMMON /C9/ NSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO, MWV
      REAL*4 GRTOL, GRSTEP, CNTOL, NSTEPV, KSTEP, CSIM,
     &       CSCM, CELLM, NLEVEL, CAVG, PPINT
      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL, TM, PINT, FPLASM, FAREA,
     &        COLNUM, ITEMAX, STAGEV, LVLCNT, GRPTI, CELLI
      REAL*4 SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO, ACPO,
     &       LCO, RIO, RCO, RBO, GTORT

*     ROUTINE VARIABLES.

      REAL*4 TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO,
     &       TTIME, TSTEP, PTEST,
     &       FLUXMM(0:NGRPTS), FLUXPM(NCELLS, 2),
     &       PDTM(0:NGRPTS), CVTDM(7, NCELLS), SPTDM(6, NCELLS),
     &       VELGRV(0:NGRPTS), VELV(0:NGRPTS),
     &       FLUXAM(2, 0:NGRPTS, 3), GAMA,
     &       CRM2TV, CRM1TV, CBTV,
     &       CMM1TM(NGRPTS-(2*(NCELLS+1))),
     &       CMTM(NGRPTS-(2*(NCELLS+1))),
     &       CMP1TM(NGRPTS-(2*(NCELLS+1))),
     &       CIM2TM(NCELLS-1), CIM1TM(NCELLS-1),
     &       CITM(NCELLS-1), CIP1TM(NCELLS-1),
     &       CIP2TM(NCELLS-1), COTV, C1TV,
     &       C2TV, OLDCIM(0:NGRPTS), CTEST

      INTEGER PCNT, ITECNT, TIM

*     STARTING THE INTERNAL CLOCK.

          CALL TIME(0,0,0)

*     INPUT DATA AND EVALUATE ALL CONSTANTS TO BE USED THROUGHOUT
*     THE PROGRAM.

      CALL INIT(TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO)

*     THE FLAG INDICATES IF THE INITIAL TIME IS STARTING FROM
*     ANOTHER VALUE THAN ZERO.

      IF(TM .EQ. 1) THEN
      READ(3,*) NLEVEL
      READ(3,*) TTIME
      READ(3,*) TSTEP
      READ(3,*) KSTEP
      READ(3,*) LVLCNT
      READ(3,*) PCNT
      READ(3,*) PTEST
      READ(3,*) ITECNT

      DO 11 K = 1, CELNUM
      READ(3,*) STAGEV(K)
11    CONTINUE

      DO 12 J = 0, RNUMEX
      DO 12 K = 1, 3
      READ(3,*) CSIM(J, K)
12    CONTINUE

      DO 13 J = 1, CELNUM
      DO 13 K = 1, 3
      READ(3,*) CSCM(1, J, K)
      READ(3,*) CSCM(2, J, K)
      READ(3,*) CSCM(3, J, K)
      READ(3,*) CSCM(4, J, K)
13    CONTINUE

      DO 14 J = 1, CELNUM
      DO 14 K =1, 3
      READ(3,*) CELLM(1, J, K)
      READ(3,*) CELLM(2, J, K)
      READ(3,*) CELLM(3, J, K)
      READ(3,*) CELLM(4, J, K)
      READ(3,*) CELLM(5, J, K)
      READ(3,*) CELLM(6, J, K)
      READ(3,*) CELLM(7, J, K)
      READ(3,*) CELLM(8, J, K)
      READ(3,*) CELLM(9, J, K)
14    CONTINUE

      ELSE

*     INITIALIZE COUNTERS AND DATA MATRICES.
```

```
      PTEST = 1.0
      ITECNT = 1

*     ALL CELLS ARE INITIALLY AT FULL TURGOR.

      DO 10 K = 1, CELNUM
         STAGEV(K) = 1
 10   CONTINUE

*     INITIALIZATION OF THE MATRIX OF INTERSTITIUM
*     CONCENTRATION OF SUCROSE.

      DO 30 J = 0, RNUMEX
      DO 30 K = 1, 3
         CSIM(J, K) = CSIOV
 30   CONTINUE

*     INITIALIZATION OF THE MATRIX OF WATER CONCENTRATION
*     IN THE CELLULAR VOLUME.

      DO 40 J = 1, CELNUM
      DO 40 K = 1, 3
         CSCM(1, J, K) = XTO
         CSCM(2, J, K) = XSTO
         CSCM(3, J, K) = XPO
         CSCM(4, J, K) = XVO
 40   CONTINUE

*     INITIALIZATION OF THE MATRIX OF CELL MENSURATIONS.

      DO 50 J = 1, CELNUM
      DO 50 K = 1, 3
         CELLM(1, J, K) = VCO
         CELLM(2, J, K) = VIO
         CELLM(3, J, K) = VTO
         CELLM(4, J, K) = RCO
         CELLM(5, J, K) = RIO
         CELLM(6, J, K) = RBO
         CELLM(7, J, K) = LCO
         CELLM(8, J, K) = AIO
         CELLM(9, J, K) = IRESPO
 50   CONTINUE

      ENDIF

 60   CONTINUE

*     COMPUTE ALL NECESSARY INFORMATION TO EVALUATE NON-LINEAR
*     COEFFICIENTS OF FINITE DIFFERENCE EQUATIONS.

      CALL PREP(FLUXMM, FLUXPM, PDTM, CVTOM, GPTOM, VELGRV,
     &          VELV, FLUXAM)

*     OUTPUT CURRENT STATE OF THE TISSUE IF DESIRED.

      IF ((TTIME .EQ. 0.0) .OR. (TTIME .GE. PTEST)) THEN
          CALL OUTPUT(TTIME, TSTEP, TMAX, FLUXMM,
     &           FLUXPM, VELV, FLUXAM, PCNT, PTEST, ITECNT)
          PCNT = PCNT + 1
          PTEST = TPRINT * REAL(PCNT)
      END IF

*     TERMINATE INTEGRATION IF FINAL TIME LEVEL REACHED.

      IF (TTIME .GE. TMAX) GO TO 999

*     EVALUATE NON-LINEAR COEFFICIENTS OF FINITE DIFFERENCE
*     EQUATIONS.

      CALL NLCOEF(VELGRV, VELV, CVTOM, GPTOM, GAMA, CRM2TV,
     &            CRM1TV, CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM,
     &            CIM1TM, CITM, CIP1TM, CIP2TM, COTV, C1TV, C2TV)

      IF (LVLCNT .EQ. 1) THEN

*       ESTIMATE CONDITION OF THE TISSUE FOR TIME LEVEL N+1/2.

        LVLCNT = 2

*       ESTIMATE INTERSTITIUM SOLUTE CONCENTRATIONS.

        CALL CSINAF(PDTM, GAMA, CRM2TV, CRM1TV, CBTV,
     &              CMM1TM, CMTM, CMP1TM, CIM2TM, CIM1TM, CITM,
     &              CIP1TM, CIP2TM, COTV, C1TV, C2TV)

 110    CONTINUE

        DO 70 J = 0, RNUMEX
           OLDCIM(J) = CSIM(J, LVLCNT+1)
 70     CONTINUE

*       ESTIMATE CELL CONDITIONS AT THE N+1/2 TIME LEVEL.

        CALL CELLCH(*999)

        TTIME = NLEVEL
        TSTEP = KSTEP

        GO TO 60

      ELSE

*       ESTIMATE CONDITION OF THE TISSUE FOR TIME LEVEL N+1.

        LVLCNT = 3

*       ESTIMATE INTERSTITIUM SOLUTE CONCENTRATIONS.

        CALL CSINP1(PDTM, GAMA, CRM2TV, CRM1TV, CBTV,
     &              CMM1TM, CMTM, CMP1TM, CIM2TM, CIM1TM, CITM,
     &              CIP1TM, CIP2TM, COTV, C1TV, C2TV)

        DO 80 J = 0, RNUMEX

*       TESTING THE CONVERGENCE
```

```
              IF (ITECNT .GT. ITEMAX) THEN
                WRITE(2, *)
                WRITE(2, *) ' ******************************'
                WRITE(2, *) ' *        >>> WARNING <<<      *'
                WRITE(2, *) ' *    NO CONVERSENCE IN C-N    *'
                WRITE(2, *) ' *          ALGORITHM.         *'
                WRITE(2, *) ' ******************************'

                GO TO 666
              END IF

              LVLCNT = 2

*             GET NEW ESTIMATES OF INTERSTITIUM CONCENTRATIONS AT
*             THE N+1/2 TIME LEVEL.

              DO 100 L = 0, RNUMEX
                CSIM(L, LVLCNT) = 0.5 * (CSIM(L, LVLCNT+1) +
     &                                   CSIM( L, LVLCNT-1))
 100           CONTINUE

              NLEVEL = NLEVEL - (0.5 * KSTEP)
              ITECNT = ITECNT + 1
              GO TO 110

            END IF

 90       CONTINUE

*         ESTIMATE CELL CONDITIONS AT THE N+1 TIME LEVEL.

          CALL CELLCH(*666)

          TTIME = NLEVEL
          TSTEP = KSTEP

*         INCREASE REDUCED TIME STEP AFTER REACHING 10S
*         BY TWO AND AFTER REACHING 20S BY TWO AGAIN

          IF(TTIME .GE. 10.0) THEN
          KSTEP = 10.0
          TSTEP = 10.0
          ELSE
          ENDIF

          IF (TTIME .GE. 20.0) THEN
          KSTEP = 20.0
          TSTEP = 20.0
          ELSE
          ENDIF

*         TRANSFER, IN THE INFORMATION MATRICES, ALL ADVANCE TIME
*         LEVEL VALUES FROM THEIR N+1 TIME LEVEL POSITION TO THEIR
*         N TIME LEVEL POSITION.

          DO 120 J = 0, RNUMEX
             CSIM(J, LVLCNT-2) = CSIM(J, LVLCNT)
 120      CONTINUE

          DO 130 J = 1, CELNUM
             CSCM(1, J, LVLCNT-2) = CSCM(1, J, LVLCNT)
             CSCM(2, J, LVLCNT-2) = CSCM(2, J, LVLCNT)
             CSCM(3, J, LVLCNT-2) = CSCM(3, J, LVLCNT)
             CSCM(4, J, LVLCNT-2) = CSCM(4, J, LVLCNT)
 130      CONTINUE

          DO 140 J = 1, CELNUM
          DO 140 I = 1, 9
             CELLM(I, J, LVLCNT-2) = CELLM(I, J, LVLCNT)
 140      CONTINUE

          LVLCNT = 4
          ITECNT = 1

          GO TO 60

        END IF

 666   CONTINUE

       CALL TIME(1,0,TIM)
       WRITE(2,1000) 'CPU TIME(MILLISECONDS)= ', TIM
 1000  FORMAT(//,T4,A,I13)
       STOP
       END

**********************************************************************
*                          SUBROUTINE INIT                           *
**********************************************************************
*                                                                    *
*  PURPOSE   - THIS SUBROUTINE INPUTS THE DATA AND EVALUATES ALL     *
*              THE CONSTANTS TO BE USED BY THE PROGRAM.              *
*                                                                    *
*  USAGE  - CALL INIT(TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO)          *
*                                                                    *
*  ARGUMENTS AND VARIABLES                                           *
*                                                                    *
*           TSTEPO - INITIAL TIME STEP FOR CRANK-NICOLSON            *
*                    INTEGRATION ROUTINE, IN SEC.                    *
*           TSTEPM - MAXIMUM TIME STEP ALLOWED IN CRANK-NICOLSON     *
*                    INTEGRATION ROUTINE, IN SEC.                    *
*             TMAX - FINAL TIME OF INTEGRATION OF CRANK-NICOLSON     *
*                    INTEGRATION ROUTINE, IN SEC.                    *
*           TPRINT - TIME INTERVAL AT WHICH PRINTOUT OF RESULTS OF   *
*                    PROGRAM CALCULATIONS IS DESIRED, IN SEC.        *
*           IRESFO - INITIAL RESISTANCE FACTOR OF THE INTERSTITIUM   *
*                    COMPLEX (DIMENSIONLESS).                        *
*             PMVV - VECTOR OF THE PARTIAL MOLAR VOLUMES OF THE      *
*                    SYSTEM SPECIES (WATER AND ALL SOLUTES), IN      *
*                    CM3 MOL-1.                                      *
*              MWV - VECTOR OF MOLECULAR WEIGHTS OF SYSTEM SPECIES,  *
*                    IN G MOL-1 (WATER, SUCROSE).                    *
*            DIFCV - PSEUDO-BINARY DIFFUSION COEFFICIENT             *
*                    OF OSMOTICUM AND INTERSTITIUM SOLUTES IN        *
*                    WATER AT INFINITE DILUTION, IN CM2 SEC-1        *
*                     DIFFUSIVITIES EXPRESSED IN CM2 SEC-1 USING       *
*                     CONCENTRATIONS IN G CM-3.                        *
*              TEMP - TEMPERATURE AT WHICH PROCESS OCCURS. ASSUMED     *
*                     TO STAY CONSTANT, IN CELSIUS.                    *
*                 R - UNIVERSAL GAS CONSTANT IN DYNE CM MOL-1 K-1      *
*             CSBOV - VECTOR OF INITIAL OSMOTICUM SOLUTE               *
*                     CONCENTRATIONS, IN G CM-3                        *
*             TSAREA - THE TOTAL SURFACE AREA OF TISSUE (TSAREA) IS    *
*                     EXPOSED TO THE OSMOTICUM, IN CM2.                *
*            THICKO - INITIAL TISSUE THICKNESS, IN CM. NOTE THAT THE   *
*                     TISSUE MUST BE AT LEAST 2 CELLS THICK.           *
*                     FOR A SEMI-INFINITE MEDIUM, THE THICKNESS IS     *
*                     DEFINED AS A FINITE DISTANCE FROM THE SURFACE    *
*                     CHOSEN SUCH THAT THE CONDITIONS THERE REMAIN     *
*                     CONSTANT AND EQUAL TO THE INITIAL VALUES         *
*                     DURING THE ENTIRE DURATION OF THE DEHYDRATION    *
*                     PROCESS.                                         *
*            DIAMCO - INITIAL AVERAGE DIAMETER OF THE CELLS IN THE     *
*                     TISSUE (SPHERE DELIMITED BY PLASMALEMMA),        *
*                     IN CM.                                           *
*             GTORT - GEOMETRICAL TORTUOSITY FACTOR (DIMENSIONLESS).   *
*      SPVFO, WVFO - INITIAL EXTRACELLULAR OPEN SPACE AND CELL WALL    *
*                     VOLUME FRACTIONS (DIMENSIONLESS).                *
*             WRESF - CELL WALL RESISTANCE FACTOR (DIMENSIONLESS).     *
*            RPLASM - RATIO OF CELL MEMBRANE SURFACE AREA OCCUPIED     *
*                     BY PLASMODESMATA (DIMENSIONLESS).                *
*            EMODCO - COEFFICIENTS OF THE LINEAR                       *
*                     FUNCTION DESCRIBING THE PRESSURE DEPENDENCE      *
*                     OF THE ELASTIC MODULUS. 2 VALUES REQUIRED:       *
*                     A (DIMENSIONLESS) AND B IN DYNES/CM2             *
*            COMPFV - VECTOR OF COMPLIANCE FACTOR VALUES RELATED TO    *
*                     EACH STAGE OF DEHYDRATION (DIMENSIONLESS).       *
*               PMV - WATER PERMEABILITY COEFFICIENT OF THE            *
*                     PLASMALEMMA MEMBRANE, IN CM/SEC.                 *
*               PPV - WATER PERMEABILITY COEFFICIENT OF THE            *
*                     PLASMODESMATA, IN CM/SEC.                        *
*             CSCOV - VECTOR OF INITIAL CELL WATER  CONCENTRATIONS,    *
*                     IN G CM-3.                                       *
*             MG,MF - MOLECULAR WEIGHT OF THE SMALL SOLUTES PRESENT    *
*           MKP,MKS   IN THE VACUOLE.                                  *
*      WG,WF,WS,WKP - WEIGHT FRACTION OF COMPONENTS IN THE             *
*       WKS,WST,WP    INTRACELLULAR VOLUME ON A DRY MATTER BASIS.      *
*            DDM,DW - DENSITY OF DRY MATTER AND DENSITY OF WATER.      *
*               PCO - HYDROSTATIC PRESSURE OF THE CELLULAR VOLUME      *
*                     AT FULL TURGOR IN DYNE CM-2                      *
*            FPLASM - FLAG TO INDICATE IF THE SYMPLAST TRANSPORT       *
*                     IS CONSIDERED.                                   *
*             FAREA - FLAG TO INDICATE IF THE AREA IS                  *
*                     ALLOWED TO VARY.                                 *
*             CSIOV - INITIAL INTERSTITIUM SUCROSE CONCENTRATION       *
*                     IN G CM-3.                                       *
*    CNTOL, ITEMAX - TOLERANCE FOR CONVERGENCE TEST IN ESTIMATION      *
*                     OF NON-LINEAR TERMS IN CRANK-NICOLSON            *
*                     ALGORITHM AND MAXIMUM NUMBER OF ITERATIONS       *
*                     ALLOWED TO CONVERGE.                             *
*            GRPCEL - NUMBER OF SPACE GRID POINTS PER CELL. DUE TO     *
*                     CERTAIN FEATURES OF THE ALGORITHM, THIS          *
*                     NUMBER MUST BE GREATER THAN OR EQUAL TO 7        *
*                     (MAXIMUM VALUE OF 10).                           *
*                PI - PI CONSTANT (DIMENSIONLESS).                     *
*               VCO - INITIAL CELLULAR VOLUME, IN CM3.                 *
*               VTO - INITIAL TOTAL UNIT CELL VOLUME, IN CM3.          *
*               VIO - INITIAL INTERSTITIUM VOLUME, IN CM3.             *
*              ACMO - CELL MEMBRANE (PLASMALEMMA) SURFACE              *
*                     AREA, IN CM2.                                    *
*              ACPO - PLASMODESMAL TRANSFER AREA BETWEEN               *
*                     2 NEIGHBOURING CELLS, IN CM2.                    *
*               LCO - INITIAL LENGTH OF EQUIVALENT CYLINDRICAL UNIT    *
*                     CELL, IN CM.                                     *
*               RIO - INITIAL INTERSTITIUM CYLINDER RADIUS, IN CM.     *
*               RCO - INITIAL CELL CYLINDER RADIUS, IN CM.             *
*               RBO - INITIAL BUFFER CYLINDER RADIUS, IN CM.           *
*               AIO - INITIAL INTERSTITIUM APOPLASTIC TRANSFER AREA,   *
*                     IN CM2.                                          *
*            DIAMTO - INITIAL DIAMETER OF THE AVERAGE UNIT CELL,       *
*                     IN CM.                                           *
*            TOTCEL - TOTAL NUMBER OF CELLS IN THE STUDIED TISSUE.     *
*            CELNUM - NUMBER OF UNITS IN THE LINEAR ARRANGEMENT OF     *
*                     EQUIVALENT CYLINDRICAL CELLS THAT FORMS THE      *
*                     MODEL COLUMN.                                    *
*                     THIS VALUE CORRESPONDS TO THE THICKNESS          *
*                     OF THE STUDIED TISSUE DIVIDED BY THE INITIAL     *
*                     AVERAGE DIAMETER OF THE AVERAGE UNIT CELL. IT    *
*                     IS THEREFORE ASSUMED THAT THESE SPHERICAL        *
*                     UNITS HAVE A CUBIC ARRANGEMENT IN THE TISSUE.    *
*            COLNUM - NUMBER OF EQUIVALENT CYLINDRICAL CELL COLUMNS    *
*                     PRESENT IN THE STUDIED TISSUE.                   *
*                     THIS VALUE CORRESPONDS TO THE NUMBER OF          *
*                     COLUMNS NECESSARY TO ENSURE THAT THE PRODUCT     *
*                     OF THE UNIT AVERAGE CELL VOLUME BY THE TOTAL     *
*                     NUMBER OF CELLS IS EQUIVALENT TO THE TOTAL       *
*                     VOLUME OF THE STUDIED TISSUE (USING THE          *
*                     CORRECTED THICKNESS).                            *
*              RNUM - TOTAL NUMBER OF GRID POINTS IN CRANK-NICOLSON    *
*                     SPACE GRID.                                      *
*            RNUMEX - TOTAL NUMBER OF POINTS IN THE EXTENDED SPACE     *
*                     GRID.                                            *
*  PLEASE NOTE THAT GRTOL, GRSTEP ARE NOT USED IN THIS PROGRAM         *
************************************************************************

      SUBROUTINE INIT(TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELL
      COMMON /C6/ GRTOL, GRSTEP, CNTOL, ITEMAX
      COMMON /C8/ NSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &            CELLM(8, NCELLS, 3), STAGEV(NCELLS),CAVG
      COMMON /C14/ DIFCV, DEGV, POLCOM(0:1)
      COMMON /C15/ COMPFV(3)
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT
      COMMON /C17/ WG,WF,WS,WKP,WKS,WST,WP,MG,MF,MKP,MKS
      COMMON /C20/ DDM,DW

      REAL*4 PMVV, RT, PMV, PPV,
     &       CDIFCM, SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &       ACPO, LCO, RIO, RCO, RSO, STORT, CAVG,
     &       EMODCO,WRESF,PCO, GRTOL, GRSTEP, CNTOL, NSTEPV, KSTEP,
     &       CSIM, CSCM, CELLM, DIFCV, POLCOM, COMPFV, DDM, DW

      REAL*4 CSSOV, CSIOV, XTO, XSTO, XPO, XVO, MWV,
     &       WG,WF,WS,WKP,WKS,WST,WP,~~MG,MF,MKP,MKS,~~ PPINT

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, ITEMAX, STAGEV, DEGV, FPLASM, FAREA,
     &        TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 TEMP, R, TSAREA, THICKO, DIAMCO, RPLASM, PI
      DATA PI/3.14159/

      INTEGER TOTCEL

      REAL*4 DIAMTO

*     INPUT DATA.

*     SOLUTION CHARACTERISTICS.

      READ(1, *) (PMVV(I), I = 1, 2)
      WRITE(2, *) ' PMVV: ', (PMVV(I), I = 1, 2)
      READ(1, *) (MWV(I), I = 1, 2)
      WRITE(2, *) ' MWV: ', (MWV(I), I = 1, 2)
        READ(1, *) DIFCV, DEGV, (POLCOM(J), J = 0, DEGV)
        WRITE(2, *) ' DIFCV, DEGV, POLCOM: ', DIFCV, DEGV,
     &               (POLCOM(J), J = 0, DEGV)

*     OSMOTICUM CHARACTERISTICS.

      READ(1, *) TEMP, R
      WRITE(2, *) ' TEMP, R: ', TEMP, R
*
*     EVALUATE THE RT CONSTANT.
      RT = R * (TEMP + 273.15)
      WRITE(2,*) ' RT: ',RT
      READ(1,*) CSSOV
      WRITE(2,*) ' CSSOV: ',CSSOV

*     INITIAL TISSUE CHARACTERISTICS (FULL TURGOR TISSUE).

      READ(1, *) TSAREA, THICKO, DIAMCO
      WRITE(2, *) ' SEMI-INFINITE MEDIUM GEOMETRY CONSIDERED.'
      WRITE(2, *) ' TSAREA, THICKO, DIAMCO: ', TSAREA, THICKO,
     &            DIAMCO
      READ(1, *) STORT, SPVFO, WVFO
      WRITE(2, *) ' STORT, SPVFO, WVFO: ', STORT, SPVFO, WVFO

*     CALCULATE THE INITIAL TISSUE VOID FRACTION.
      VOIDFO = SPVFO + WVFO
      WRITE(2,*) ' VOIDFO: ',VOIDFO

      READ(1,*) FPLASM
         IF(FPLASM .EQ. 1) THEN
            WRITE(2,*) ' SYMPLAST TRANSPORT IS CONSIDERED.'
         ELSE
            WRITE(2,*) ' SYMPLAST TRANSPORT IS NOT CONSIDERED.'
         ENDIF
      READ(1,*) FAREA
         IF(FAREA .EQ. 1) THEN
            WRITE(2,*) ' THE AREA OF EXTRACELLULAR SPACE VARIES'
         ELSE
            WRITE(2,*) ' THE AREA OF EXTRACELLULAR SPACE IS FIXED'
         ENDIF

*     CELL CHARACTERISTICS.

      READ(1, *) WRESF, RPLASM
      WRITE(2, *) ' WRESF, RPLASM: ', WRESF, RPLASM

*     CALCULATE THE INITIAL RESISTANCE OF THE INTERSTITIUM COMPLEX.
      IRESFO = (SPVFO + (WVFO * WRESF)) / VOIDFO
      WRITE(2,*) ' IRESFO: ',IRESFO

      READ(1, *) (EMODCO(K), K = 1, 2)
      WRITE(2, *) ' LINEAR VARIATION OF ELASTIC MODULUS',
     &            ' CONSIDERED: ', (EMODCO(K), K = 1, 2)
      READ(1,*) PCO
      WRITE(2,*) ' PCO: ',PCO
      READ(1, *) (COMPFV(K), K = 1, 3)
      WRITE(2, *) ' COMPLIANCE FACTOR VALUES: ',
     &           (COMPFV(K), K = 1, 3)
      READ(1, *) PMV
      WRITE(2, *) ' PMV: ', PMV
      READ(1, *) PPV
      WRITE(2, *) ' PPV: ', PPV
      READ(1, *) XTO, XSTO, XPO, XVO
      WRITE(2, *) ' XTO: ', XTO,' XSTO: ',XSTO,' XPO: ',XPO,
     &            ' XVO: ', XVO
      READ(1,*) WG,WF,WS,WKP,WKS,WST,WP
      WRITE(2,*) ' WG: ',WG,' WF: ',WF,' WS: ',WS,' WKP: ',WKP,
     &            ' WKS: ',WKS,' WST: ',WST,' WP: ',WP
      READ(1,*) MG,MF,MKP,MKS
      WRITE(2,*) ' MG: ',MG,' MF: ',MF,' MKP: ',MKP,' MKS: ',MKS
      READ(1,*) DDM,DW
      WRITE(2,*) ' DDM: ',DDM,' DW:',DW

*     INTERSTITIUM CHARACTERISTICS.
```

```
      CAVE = (((1.0029 + (0.3599 * CSIOV)) +
     &        (1.0029 + (0.3599 * CSBOV))) / 2
      WRITE(2,*) ' CAVE: ', CAVE

*     PARAMETERS REQUIRED BY GEARS AND CRANK-NICOLSON ROUTINES.

      READ(1, *) GRTOL, GRSTEP, CNTOL, ITEMAX
      WRITE(2, *) ' GRTOL, GRSTEP, CNTOL, ITEMAX: ', GRTOL, GRSTEP,
     &            CNTOL, ITEMAX
      READ(1, *) GRPCEL
      WRITE(2, *) ' GRPCEL: ', GRPCEL
      READ(1, *) TSTEPO, TSTEPM, TMAX, TPRINT
      WRITE(2, *) ' TSTEPO, TSTEPM, TMAX, TPRINT: ', TSTEPO, TSTEPM,
     &            TMAX, TPRINT
      READ(1, *) TM, PINT, PPINT
      WRITE(2, *) ' TM, PINT, PPINT: ', TM, PINT, PPINT

*     GET INITIAL EQUIVALENT CYLINDRICAL UNIT CELL MENSURATIONS.

*     INITIAL CELLULAR VOLUME.

      DATA PI/3.14159/
      VCO = (PI * (DIAMCO**3)) / 6.0

*     INITIAL TOTAL UNIT CELL VOLUME.

      VTO = VCO / (1.0 - VOIDFO)

*     INITIAL INTERSTITIUM VOLUME.

      VIO = VTO - VCO
      WRITE(2, *) ' VCO, VIO, VTO: ', VCO, VIO, VTO

*     INITIAL CELL MEMBRANE SURFACE AREA.

      ACMO = (1.0 - RPLASM) * PI * (DIAMCO**2)

*     INITIAL FRACTIONAL PLASMODESMAL TRANSFER AREA.

*     NOTE:  THE TERM "PLASMODESMAL TRANSFER AREA" USED
*            THROUGHOUT THE PROGRAM REFERS TO THE FRACTION OF
*     TOTAL PLASMODESMAL AREA WHICH IS USED, FOR ANY GIVEN CELL,
*     TO DESCRIBE THE SURFACE AVAILABLE FOR SYMPLASTIC TRANSPORT
*     TO/FROM ADJOINING CELLS. THIS FRACTION IS ASSUMED EQUAL FOR
*     ALL 6 POINTS OF CONTACT.

      ACPO = (RPLASM * ACMO) / (6.0 * (1.0 - RPLASM))

*     INITIAL LENGTH OF UNIT CYLINDRICAL CELL.

      LCO = (8.0 * VTO * (GTORT**(3.0 / 2.0)) / PI)**(1.0 / 3.0)

*     INITIAL RADIUS OF INTERSTITIUM CYLINDER.

      RIO = ACMO / (2.0 * PI * LCO)

*     INITIAL CELL CYLINDER RADIUS.

      RCO = SQRT((VCO / (PI * LCO)) + (RIO**2))

*     INITIAL BUFFER CYLINDER RADIUS.

      RBO = SQRT((RIO**2) - (VIO / (PI * LCO)))
      WRITE(2, *) ' LCO, RIO, RCO, RBO: ', LCO, RIO, RCO, RBO

*     INITIAL INTERSTITIUM APOPLASTIC TRANSFER AREA.

      AIO = PI * ((RIO**2) - (RBO**2))
      WRITE(2, *) ' AIO, ACMO, ACPO: ', AIO, ACMO, ACPO

*     DEFINE SOME PARAMETERS TO BE USED BY CRANK-NICOLSON ALGORITHM.

*     GET INITIAL AVERAGE UNIT CELL DIAMETER.

      DIAMTO = (6.0 * VTO / PI)**(1.0 / 3.0)
      WRITE(2, *) ' DIAMTO: ', DIAMTO

*     EVALUATE TOTAL NUMBER OF CELLS IN TISSUE.

      TOTCEL = INT((TSAREA * THICKO / VTO) + 1.0)
      WRITE(2, *) ' TOTCEL: ', TOTCEL

*     EVALUATE NUMBER OF EQUIVALENT CYLINDRICAL UNIT CELLS IN
*     MODEL COLUMN.

*     CELNUM IS TAKEN AS THE NEAREST INTEGER GREATER THAN
*     THE CALCULATED VALUE (SEE CELNUM DEFINITION).

      CELNUM = INT((THICKO / DIAMTO) + 1.0)

*     EVALUATE NUMBER OF COLUMNS IN THE STUDIED TISSUE.

      COLNUM = TOTCEL / CELNUM

*     EVALUATE TOTAL NUMBER OF SPACE GRID POINTS (FOR BOTH SPACE
*     GRIDS).

      RNUM = (CELNUM * GRPCEL) - CELNUM
      RNUMEX = (CELNUM * GRPCEL) - 1
      WRITE(2, *) ' CELNUM, COLNUM, RNUM, RNUMEX: ', CELNUM, COLNUM,
     &            RNUM, RNUMEX

      END

*******************************************************************
*                        SUBROUTINE PREP                          *
*******************************************************************
*                                                                 *
*  PURPOSE  - THIS SUBROUTINE IS USED TO ESTIMATE THE INFORMATION *
*             NECESSARY TO EVALUATE THE NON-LINEAR COEFFICIENTS   *
*             OF THE FINITE DIFFERENCE EQUATIONS.                 *
*                                                                 *
*  USAGE  - CALL PREP(FLUXMM, FLUXPM, PDTM, CYTOM, GPTOM, VELGRV,  *
*                     VELV, FLUXAM)                               *
*                                                                 *
*  ARGUMENTS AND VARIABLES                                        *
*                                                                 *
*        FLUXPM - MATRIX OF WATER PLASMODESMATAL FLUXES, IN         *
*                 G CM-2 SEC-1.                                     *
*          PDTM - VECTOR OF WATER PRODUCTION DEPLETION TERMS        *
*         GPTOM - MATRIX OF GEOMETRICAL AREA OF EXTRACELLULAR       *
*                 SPACE TIME DERIVATIVES.                           *
*        VELGRV - VECTOR OF MASS AVERAGE VELOCITY GRADIENTS.        *
*          VELV - VECTOR OF MASS AVERAGE VELOCITIES.                *
*        FLUXAM - MATRIX OF APOPLASTIC FLUXES.                      *
*         CELLI - CELL POSITION INDEX.                              *
*        GRPCNT - SPACE GRID POINT COUNTER.                         *
*         GRPTI - SPACE GRID POINT POSITION INDEX.                  *
*           PSI - VARIABLE USED IN CALCULATION OF THE               *
*                 PRODUCTION-DEPLETION TERMS.                       *
*    SUM1, SUM2 - SUMMATION VARIABLES.                              *
*********************************************************************

      SUBROUTINE PREP(FLUXMM, FLUXPM, PDTM, CVTOM, GPTOM, VELGRV,
     &                VELV, FLUXAM)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3600, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 FLUXMM(0:NGRPTS), FLUXPM(NCELLS, 2),
     &       PDTM(0:NGRPTS), CVTOM(3, NCELLS), GPTOM(6, NCELLS),
     &       VELGRV(0:NGRPTS), VELV(0:NGRPTS),
     &       FLUXAM(2, 0:NGRPTS, 3)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, STORT
      COMMON /C9/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 PMVV, RT, PMV, PPV,
     &       SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &       ACPO, LCO, RIO, RCO, RBO, STORT, HSTEPV, KSTEP,
     &       CSIM, CSCM, CELLM, NLEVEL, CAVG

      REAL*4  CSBOV, CSIOV, XTO, XSTO, XPO, XVO, PPINT

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 PI

      DATA PI/3.14159/

      REAL*4 PSI, SUM1, SUM2

      INTEGER GRPCNT, FPLASM, FAREA

*     COMPUTE CURRENT VALUES OF SPACE STEPS (FOR ALL CELLS).

      DO 10 J = 1, CELNUM
         HSTEPV(J) = CELLM(7, J, LVLCNT) / REAL(GRPCEL - 1)
 10   CONTINUE

*     GET ESTIMATES OF THE LOCAL CORRECTED PSEUDO-BINARY DIFFUSION
*     COEFFICIENT.

      DO 20 J = 1, CELNUM
         CELLI = J
         CALL DCFUNC
 20   CONTINUE

*     EVALUATE LOCAL TRANSMEMBRANE FLUXES (FOR WATER AND ALL
*     EXTENDED SPACE GRID POINTS, ON A CELL BY CELL BASIS).

      CELLI = 1
      GRPCNT = 1
      DO 30 J = RNUMEX, 0, -1
         GRPTI = J
         CALL FLUXM(FLUXMM)
         IF (GRPCNT .GE. GRPCEL) THEN
           CELLI = CELLI + 1
           GRPCNT = 1
          ELSE
           GRPCNT = GRPCNT + 1
         END IF
 30   CONTINUE

*     FLAG TO INDICATE IF THE PLASMODESMAL FLUXES
*     WILL BE CONSIDERED

      IF(FPLASM .EQ. 1 ) THEN

*     EVALUATE, FOR EACH CELL, THE PLASMODESMAL FLUXES.

      DO 40 J = 1, CELNUM+1
         CELLI = J
         CALL FLUXP(FLUXPM)
 40   CONTINUE

      ELSE

      DO 45 J = 1, CELNUM+1
         CELLI = J
         FLUXPM(CELLI, 1) = 0
         FLUXPM(CELLI, 2) = 0
 45   CONTINUE

*     [illegible] ON A CELL BY CELL BASIS, THE LOCAL PRODUCTION
```

```
      GRPCNT = 1
      GRPTI = RNUMEX

 70    CONTINUE

      PSI = (2*PI*CELLM(5,CELLI,LVLCNT))/CELLM(8,CELLI,LVLCNT)

 80    CONTINUE

*     GET LOCAL WATER PRODUCTION-DEPLETION TERM.

        PDTM(GRPTI) = PSI * FLUXMM(GRPTI)

      IF (GRPTI .LE. 0 ) THEN
        GO TO 90
       ELSE
        GRPTI = GRPTI - 1
      END IF

      IF (GRPCNT .GE. GRPCEL) THEN
        CELLI = CELLI + 1
        GRPCNT = 1
        GO TO 70
       ELSE
        GRPCNT = GRPCNT + 1
        GO TO 80
      END IF

 90    CONTINUE

*     EVALUATE, FOR EACH CELL, THE CURRENT CELLULAR, INTERSTITIUM
*     AND TOTAL CELL VOLUME TIME DERIVATIVES.

      DO 100 J = 1, CELNUM
         CELLI = J
         CALL CVFUNC(FLUXMM, FLUXPM, CVTDM)
 100   CONTINUE

*     EVALUATE, FOR EACH CELL, THE CURRENT GEOMETRICAL TIME
*     DERIVATIVES PARAMETERS AND PARTICULARLY THE APOPLASTIC
*     TRANSFER AREA.

      DO 115 J = 1, CELNUM
         CELLI = J
         CALL GPFUNC(CVTDM, GPTDM)
 115   CONTINUE

*     EVALUATE THE LOCAL MASS AVERAGE VELOCITY GRADIENTS
*     (FOR ALL EXTENDED SPACE GRID POINTS, ON A CELL BY CELL BASIS)

      CELLI = CELNUM
      GRPCNT = 1
      DO 110 J = 0, RNUMEX

*     FLAG WHICH INDICATES IF AI VARIES ALONG THE PROCESS.

      IF(FAREA .EQ. 1) THEN

         VELGRV(J) =  (PDTM(J) / CAVC) - (GPTDM(8, CELLI) /
     &                CELLM(8, CELLI, LVLCNT))

      ELSE

         VELGRV(J)  PDTM(J) / CAVC

      ENDIF

         IF (GRPCNT .GE. GRPCEL) THEN
           CELLI = CELLI - 1
           GRPCNT = 1
          ELSE
           GRPCNT = GRPCNT + 1
         END IF

 110   CONTINUE

*     EVALUATE THE LOCAL MASS VOLUME AVERAGE VELOCITIES (ON A
*     CELL BY CELL BASIS, FOR ALL EXTENDED SPACE GRID POINTS).

*     THE BOUNDARY CONDITION AT THE CENTER IMPLIES THAT THE
*     MASS AVERAGE VELOCITY IS EQUAL TO ZERO AT ANY TIME.

      VELV(0) = 0.0

      CALL VELOCT(VELGRV, VELV)

*     EVALUATE LOCAL VALUES OF APOPLASTIC SOLUTE FLUXES.

      CALL FLUXA(VELV, FLUXAM)

      END
*****************************************************************
*                     SUBROUTINE NLCOEF                         *
*****************************************************************
*                                                               *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE NON-LINEAR COEFFICIENTS*
*             THAT APPEAR IN THE FINITE DIFFERENCE EQUATIONS AT *
*             THE N-TH TIME LEVEL AND FOR ALL SOLUTES.          *
*                                                               *
*  USAGE   - CALL NLCOEF(VELGRV, VELV, CVTDM, GPTDM, GAMA       *
*                    CRM2TV, CRM1TV, CBTV, CMM1TM, CMTM, CMP1TM, *
*                    CIM2TM, CIM1TM, CITM, CIP1TM, CIP2TM, COTV, *
*                    C1TV, C2TV)                                *
*                                                               *
*  ARGUMENTS AND VARIABLES                                      *
*                                                               *
*            VELGRV - VECTOR OF MASS AVERAGE VELOCITY           *
*                     GRADIENTS.                                *
*              VELV - VECTOR OF MASS AVERAGE VELOCITIES.        *
*             CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES. *
*             GPTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES. *
*              GAMA - COEFFICIENTS USED IN CALCULATION OF SOME  *
*                     NON-LINEAR TERMS.                         *
*   CRM2TV, CRM1TV, - NON-LINEAR COEFFICIENTS OF THE            *
*   CBTV              (R-1)-TH SPACE GRID POINT FINITE DIFFERENCE *
*                       N IS NOT AN INTERFACE POINT).                     *
*   CIM2TM, CIM1TM,  -  VECTORS OF NON-LINEAR COEFFICIENTS OF THE         *
*   CITM, CIP1TM,       I-TH INTERFACE SPACE GRID POINT FINITE            *
*   CIP2TM              DIFFERENCE EQUATIONS.                             *
*  COTV, C1TV, C2TV  -  NON-LINEAR COEFFICIENTS OF THE                    *
*                       FIRST SPACE GRID POINT FINITE DIFFERENCE          *
*                       EQUATIONS.                                        *
*    ALPHAV, BETAV,  -  COEFFICIENTS USED IN CALCULATION OF               *
*    PSI                PRECEDING NON-LINEAR TERMS.                       *
*            GRPCNT  -  SPACE GRID POINT COUNTER.                         *
*     MATI1, MATI2,  -  MATRIX COLUMN POSITION INDICES.                   *
*     MATI3                                                               *
***************************************************************************

*     SUBROUTINE NLCOEF(VELGRV, VELV, CVTDM, GPTDM, GAMA,
     &             CRM2TV, CRM1TV, CSTV, CMM1TM, CMTM, CMP1TM,
     &             CIM2TM, CIM1TM, CITM, CIP1TM, CIP2TM, COTV, C1TV,
     &             C2TV)

      INTEGER  NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4  VELGRV(0:NGRPTS), VELV(0:NGRPTS), CVTDM(3, NCELLS),
     &        GPTDM(5, NCELLS), GAMA,
     &        CRM2TV, CRM1TV, CSTV,
     &        CMM1TM(NGRPTS-(2*(NCELLS+1))),
     &        CMTM(NGRPTS-(2*(NCELLS+1))),
     &        CMP1TM(NGRPTS-(2*(NCELLS+1))),
     &        CIM2TM(NCELLS-1), CIM1TM(NCELLS-1),
     &        CITM(NCELLS-1), CIP1TM(NCELLS-1),
     &        CIP2TM(NCELLS-1), COTV, C1TV,
     &        C2TV

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELLS)
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C8/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C18/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 CDIFCM, SPVFO, WVFO, VOIDFO, VCO, VIO, VTO,
     &       AIO, ACMO, ACPO, LCO, RIO, RCO, RBO, GTORT, HSTEPV,
     &       KSTEP,CSIM, CSCM, CELLM, CAVG,
     &       NLEVEL, PPINT

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 ALPHAV(NCELLS), BETAV(NCELLS), PSI

      INTEGER GRPCNT, MATI1, MATI2, MATI3, FPLASM, FAREA

      GAMA = 0.5 * KSTEP

      DO 10 K = 1, CELNUM
         ALPHAV(K) = KSTEP / (2.0 * (HSTEPV(K)**2))
         BETAV(K) = KSTEP / (4.0 * HSTEPV(K))
 10   CONTINUE

*     EVALUATE COEFFICIENTS OF THE FIRST GRID POINT EQUATION
*     OR CENTER GRID POINT.

          COTV = (ALPHAV(CELNUM) * CDIFCM(1))+
     &                (BETAV(CELNUM) * VELV(1))

*     FLAG WHICH INDICATES IF AI VARIES ALONG THE PROCESS.

      IF(FAREA .EQ. 1) THEN

          C1TV =
     &      (ALPHAV(CELNUM) * (CDIFCM(3) + CDIFCM(1)))
     &      + (GAMA * (VELGRV(1) +
     &       (GPTDM(5, CELNUM) / CELLM(5, CELNUM, LVLCNT))))

      ELSE

          C1TV =
     &      (ALPHAV(CELNUM) * (CDIFCM(3) + CDIFCM(1)))
     &      + (GAMA * VELGRV(1))

      ENDIF

          C2TV = (ALPHAV(CELNUM) * CDIFCM(3))
     &                - (BETAV(CELNUM) * VELV(1))

 25       CONTINUE

*     EVALUATE COEFFICIENTS OF THE [illegible] TH GRID POINT EQUATION
*     OR POINT BEFORE THE SURFACE.

      MATI3 = (((GRPCE[illegible] 2) - 1) * CELNUM) - 1

          CRM2TV = (ALPHAV(1) * CDIFCM(MATI3-3)) +
     &                  (BETAV(1) * VELV(RNUMEX-1))

*     FLAG WHICH INDICATES IF AI VARIES ALONG THE PROCESS.

      IF(FAREA .EQ. 1) THEN

          CRM1TV =
     &      (ALPHAV(1) * (CDIFCM(MATI3-1) + CDIFCM(MATI3-3)))
     &      + (GAMA * (VELGRV(RNUMEX-1) + (GPTDM(5, 1) /
     &                                  CELLM(5, 1, LVLCNT))))

      ELSE
      ENDIF

         CBTV = (ALPHAV(1) * CDIFCM(MATI3-1)) -
     &              (BETAV(1) * VELV(RNUMEX-1))

*     EVALUATE COEFFICIENTS OF N-TH GRID POINT EQUATIONS (INCLUDING
*     INTERFACE POINTS).

        CELLI = CELNUM
        GRPCNT = 3
        GRPTI = 2
        MATI1 = 1
        MATI2 = 1
        MATI3 = 3

 50       CONTINUE

        IF (GRPCNT .LT. GRPCEL) THEN

          CMM1TM(MATI1) = (ALPHAV(CELLI) * CDIFCM(MATI3))+
     &                       (BETAV(CELLI) * VELV(GRPTI))

*     FLAG WHICH INDICATES IF AI VARIES ALONG THE PROCESS.

      IF(FAREA .EQ. 1) THEN

          CMTM(MATI1) =
     &      (ALPHAV(CELLI) * (CDIFCM(MATI3+2) + CDIFCM(MATI3)))
     &      + (GAMA * (VELGRV(GRPTI) +
     &        (GPTDM(6, CELLI) / CELLM(6, CELLI, LVLCNT))))

      ELSE

          CMTM(MATI1) =
     &      (ALPHAV(CELLI) * (CDIFCM(MATI3+2) + CDIFCM(MATI3)))
     &      + (GAMA * VELGRV(GRPTI))

      ENDIF

          CMP1TM(MATI1) = (ALPHAV(CELLI) * CDIFCM(MATI3+2))
     &                    - (BETAV(CELLI) * VELV(GRPTI))

          GRPCNT = GRPCNT + 1
          GRPTI = GRPTI + 1
          MATI1 = MATI1 + 1
          MATI3 = MATI3 + 2

          IF ((GRPTI .EQ. RNUMEX-1) .OR. (CELNUM .EQ. 1)) GO TO 40

          GO TO 50

        ELSE

*        INTERFACE POINT VALUES

          PSI = (CELLM(6, CELLI, LVLCNT) * CDIFCM(MATI3+1) *
     &          HSTEPV(CELLI-1)) / (CELLM(6, CELLI-1, LVLCNT) *
     &          CDIFCM(MATI3+2) * HSTEPV(CELLI))

          CIM2TM(MATI2) = PSI
          CIM1TM(MATI2) = 4.0 * PSI
          CITM(MATI2) = 3.0 + (3.0 * PSI)
          CIP1TM(MATI2) = 4.0
          CIP2TM(MATI2) = 1.0

          CELLI = CELLI - 1
          GRPCNT = 2
          GRPTI = GRPTI + 2
          MATI2 = MATI2 + 1
          MATI3 = MATI3 + 3

          GO TO 50

        END IF

 40     CONTINUE

      END
************************************************************************
*                         SUBROUTINE CSIHAF                            *
************************************************************************
*                                                                      *
*  PURPOSE   - THIS SUBROUTINE IS USED TO ESTIMATE THE                 *
*              INTERSTITIUM SUCROSE CONCENTRATION AT THE N+1/2 TIME    *
*              LEVEL.                                                  *
*                                                                      *
*  USAGE   - CALL CSIHAF(PDTM, GAMA,                                   *
*                        CRM2TV, CRM1TV,                               *
*                        CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM,           *
*                        CIM1TM, CITM, CIP1TM, CIP2TM, COTV, C1TV;     *
*                        C2TV)                                         *
*                                                                      *
*  ARGUMENTS AND VARIABLES                                             *
*                                                                      *
*               PDTM - VECTOR OF WATER PRODUCTION-DEPLETION TERM.      *
*               GAMA - COEFFICIENT  USED IN CALCULATION OF             *
*                      INTERSTITIUM CONCENTRATION  (SEE SUBROUTINE     *
*                      NLCOEF FOR DETAILS, DIMENSIONLESS).             *
*  CRM2TV, CRM1TV, CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM, CIM1TM,         *
*  CITM, CIP1TM, CIP2TM, COTV, C1TV, C2TV                              *
*                    - SCALARS AND VECTORS OF NON-LINEAR               *
*                      COEFFICIENTS OF THE FINITE DIFFERENCE           *
*                      EQUATIONS (SEE SUBROUTINE NLCOEF FOR            *
*                      DETAILS, DIMENSIONLESS).                        *
*             GRPCNT - SPACE GRID POINT COUNTER.                       *
*       MATI1, MATI2 - MATRIX COLUMN POSITION INDICES.                 *
************************************************************************

      SUBROUTINE CSIHAF(PDTM, GAMA, CRM2TV, CRM1TV,
     &                  CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM,
     &                  CIM1TM, CITM, CIP1TM, CIP2TM, COTV, C1TV,
     &                  C2TV)

      INTEGER NGRPTS, NCELLS
      REAL*4  PDTM(0:NGRPTS), GAMA,
     &        CRM2TV, CRM1TV, CBTV,
     &        CMM1TM(NGRPTS-(2*(NCELLS+1))),
     &        CMTM(NGRPTS-(2*(NCELLS+1))),
     &        CMP1TM(NGRPTS-(2*(NCELLS+1))),
     &        CIM2TM(NCELLS-1), CIM1TM(NCELLS-1),
     &        CITM(NCELLS-1), CIP1TM(NCELLS-1),
     &        CIP2TM(NCELLS-1), C0TV, C1TV,
     &        C2TV

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELLS)
      COMMON /C8/ NSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(5, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI

      REAL*4 CSIM, CSCM, CELLM, NLEVEL, CAVG, CDIFCM

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO

      REAL*4 NSTEPV, KSTEP

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

*     ROUTINE VARIABLES.

      INTEGER GRPCNT, MATI1, MATI2

*     USING INFORMATION AT THE N TIME LEVEL, ESTIMATE CONCENTRATIONS
*     AT THE FIRST AND AT THE (R-1)-TH SPACE GRID POINTS.

        CSIM(1, LVLCNT) = (C0TV *CSIOV) +
     &                    ((1.0 - C1TV) * CSIM(1, LVLCNT-1)) +
     &                    (C2TV *  CSIM(2, LVLCNT-1))

        CSIM(RNUMEX-1, LVLCNT) =
     &          (CRM2TV * CSIM(RNUMEX-2, LVLCNT-1)) +
     &          ((1.0 - CRM1TV) * CSIM(RNUMEX-1, LVLCNT-1))


        CSIM(RNUMEX-1, LVLCNT) = CSIM(RNUMEX-1, LVLCNT)
     &          + (CBTV * CSBOV)

*     ESTIMATE CONCENTRATION AT THE M-TH SPACE GRID POINT (EXCEPT
*     INTERFACE POINTS).

        GRPCNT  = 3
        GRPTI = 2
        MATI1 = 1

 30       CONTINUE

        IF (GRPCNT .LT. GRPCEL) THEN

          CSIM(GRPTI, LVLCNT) =
     &      (CMM1TM(MATI1) * CSIM(GRPTI-1, LVLCNT-1)) +
     &       ((1.0 - CMTM(MATI1)) * CSIM(GRPTI, LVLCNT-1)) +
     &      (CMP1TM(MATI1) * CSIM(GRPTI+1, LVLCNT-1))

          GRPCNT = GRPCNT + 1
          GRPTI = GRPTI + 1
          MATI1 = MATI1 + 1
          IF (GRPTI .EQ. RNUMEX-1) GO TO 20
          GO TO 30

         ELSE

          GRPCNT = 2
          GRPTI = GRPTI + 2
          GO TO 30

        END IF

 20     CONTINUE

*     ESTIMATE CONCENTRATION AT THE ZERO-TH (CENTRE) AND R-TH
*     (SURFACE) SPACE GRID POINTS.

      MATI1 = (((GRPCEL * 2) - 1) * CELNUM) - 1

          CSIM(0, LVLCNT) = CSIOV

          CSIM(RNUMEX, LVLCNT) = CSBOV

*     ESTIMATE CONCENTRATION AT THE I-TH INTERFACE POINT.

      IF (CELNUM .EQ. 1) RETURN

        GRPTI = GRPCEL - 1
        MATI2 = 1

 60       CONTINUE

        CSIM(GRPTI, LVLCNT) = - (1.0 / CITM(MATI2)) *
     &    ((CIP2TM(MATI2) * CSIM(GRPTI+3, LVLCNT)) -
     &     (CIP1TM(MATI2) * CSIM(GRPTI+2, LVLCNT)) +
     &    (CIM2TM(MATI2) * CSIM(GRPTI-2, LVLCNT)) -
     &     (CIM1TM(MATI2) * CSIM(GRPTI-1, LVLCNT)))

        CSIM(GRPTI+1, LVLCNT) = CSIM(GRPTI, LVLCNT)

        GRPTI = GRPTI + GRPCEL
        MATI2 = MATI2 + 1
      - IF (GRPTI .EQ. RNUMEX) GO TO 50
        GO TO 60

 50       CONTINUE

      DO 70 I = 0, RNUMEX
      END

***************************************************************
*                       SUBROUTINE CELLCH                     *
***************************************************************
*                                                             *
*  PURPOSE  - THIS SUBROUTINE USES A SIMPLE DISCRETIZATION    *
*             TO EVALUATE, FOR A GIVEN TIME INTERVAL (REAL TIME) *
*             AND FOR ALL CELLS SIMULTANEOUSLY, THE CHANGES IN  *
*             CELLULAR, INTERSTITIUM AND TOTAL UNIT CELL VOLUMES, *
*             THE CHANGES IN THE APOPLAST TRANSFER AREA IF DESIRED,*
*             THE CHANGES IN CELL GEOMETRICAL MENSURATIONS AND  *
*             FINALLY, THE CHANGES IN THE CELL WATER CONCENTRATION.*
*                                                             *
*  USAGE  - CALL CELLCH(*M)                                   *
*                                                             *
*  ARGUMENTS AND VARIABLES                                    *
*                                                             *
*          NCOUNT - POSITION COUNTER                          *
*          FLUXMM - VECTOR OF TRANSMEMBRANES, IN G/CM3        *
*          FLUXMP - MATRIX OF PLASMODESMAL FLUXES, IN G/CM3   *
*           CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES, *
*                   IN CM3 SEC-1                              *
*           GPTDM - MATRIX OF UNIT CELL GEOMETRICAL PARAMETER *
*                   TIME DERIVATIVES.                         *
*           CSTDM - MATRIX OF CELL WATER CONCENTRATION TIME   *
*                   DERIVATIVES IN G WATER/G DRY MATTER SEC   *
***************************************************************

      SUBROUTINE CELLCH(*)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C8/ NSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(8, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 NSTEPV, KSTEP,
     &       CSIM, CSCM, CELLM, NLEVEL, CAVG, PPINT

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI,
     &        FPLASM, FAREA, TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 T, TEND, DT

      REAL*4 FLUXMM(0:NGRPTS), FLUXPM(NCELLS, 2),
     &       CVTDM(3, NCELLS), GPTDM(6, NCELLS),
     &       CSTDM(1, NCELLS)

      INTEGER  GRPCNT

*     INITIAL VALUE OF INDEPENDENT VARIABLE, I.E., CURRENT TIME,
*     IN SEC.

      T = NLEVEL

*     TIME VALUE AT WHICH SOLUTION IS DESIRED.

      TEND = (NLEVEL + (0.5 * KSTEP))

*     CALCULATION OF DT.

      DT = TEND - T

*     EVALUATE LOCAL TRANSMEMBRANE FLUXES (FOR WATER AND ALL
*     EXTENDED SPACE GRID POINTS, ON A CELL BY CELL BASIS).

      CELLI = 1
      GRPCNT = 1
      DO 30 J = RNUMEX, 0, -1
         GRPTI = J
         CALL FLUXM(FLUXMM)
         IF (GRPCNT .GE. GRPCEL) THEN
           CELLI = CELLI + 1
           GRPCNT = 1
          ELSE
           GRPCNT = GRPCNT + 1
         END IF
 30    CONTINUE

*     EVALUATE, FOR EACH CELL, THE PLASMODESMAL FLUXES
*     IF THE FLAG INDICATES.

      IF(FPLASM .EQ. 1) THEN

      DO 40 J = 1, CELNUM+1
         CELLI = J
         CALL FLUXP(FLUXPM)
 40    CONTINUE

      ELSE

      DO 45 J = 1, CELNUM+1
         CELLI = J
         FLUXPM(CELLI, 1) = 0
         FLUXPM(CELLI, 2) = 0
 45    CONTINUE

      ENDIF

*     EVALUATE, FOR EACH CELL, THE CURRENT CELLULAR, INTERSTITIUM
*     AND TOTAL CELL VOLUME TIME DERIVATIVES.

      DO 50 J = 1, CELNUM
         CELLI = J
```

```
*     EVALUATE, FOR EACH CELL, THE CURRENT TIME DERIVATIVES OF THE
*     EQUIVALENT CYLINDRICAL UNIT CELL GEOMETRICAL PARAMETERS.

      DO 70 J = 1, CELNUM
         CELLI = J
         CALL GPFUNC(CVTDM, GPTDM)
 70    CONTINUE

*     EVALUATE THE CELL WATER CONCENTRATION TIME DERIVATIVE
*     (FOR ALL CELLS).

      DO 80 J = 1, CELNUM
         CELLI = J
         CALL CCFUNC(FLUXMM, FLUXPM, CVTDM, CSTDM)
 80    CONTINUE

*     CALCULATION OF THE NEW VALUES OF VC, VI, VT, RC, RI, RB,
*     LC, AI  AND IRESF BY FINITE DIFFERENCES FOR ALL CELLS.

      DO 100 J = 1, CELNUM

*      VC OR CELLM(1, J, LVLCNT).
            CELLM(1, J, LVLCNT) = CELLM(1, J, LVLCNT-1) +
     &                  (CVTDM(1, J) * DT)

*      VI OR CELLM(2, J, LVLCNT).
            CELLM(2, J, LVLCNT) = CELLM(2, J, LVLCNT-1) +
     &                   (CVTDM(2, J) * DT)

*      VT OR CELLM(3, J, LVLCNT).
            CELLM(3, J, LVLCNT) = CELLM(3, J, LVLCNT-1) +
     &                    (CVTDM(3, J) * DT)

*      RC OR CELLM(4, J, LVLCNT).
            CELLM(4, J, LVLCNT) = CELLM(4, J, LVLCNT-1) +
     &                    (GPTDM(3, J) * DT)

*      RI OR CELLM(5, J, LVLCNT).
            CELLM(5, J, LVLCNT) = CELLM(5, J, LVLCNT-1) +
     &                    (GPTDM(2, J) *DT)

*      RB OR CELLM(6, J, LVLCNT).
            CELLM(6, J, LVLCNT) = CELLM(6, J, LVLCNT-1) +
     &                    (GPTDM(4, J) * DT)

*      LC OR CELLM(7, J, LVLCNT).
            CELLM(7, J, LVLCNT) = CELLM(7, J, LVLCNT-1) +
     &                    (GPTDM(1, J) *DT)

*      THE TIME DERIVATIVE OF THE EXTRACELLULAR SPACE TRANSFER
*      AREA IS CALCULATED IF DESIRED.

*      AI OR CELLM(8, J, LVLCNT).

          IF (FAREA .EQ. 0) THEN
             CELLM(8, J, LVLCNT) = CELLM(8, J, LVLCNT-1)
          ELSE
             CELLM(8, J, LVLCNT) = CELLM(8, J, LVLCNT-1) +
     &                    (GPTDM(5, J) * DT)
          ENDIF

*      IRESF OR CELLM(9, J, LVLCNT).
             CELLM(9, J, LVLCNT) = CELLM(9, J, LVLCNT-1) +
     &                    (GPTDM(5, J) * DT)

*      CSCM(1, J, LVLCNT)
             CSCM(1, J, LVLCNT) = CSCM(1, J, LVLCNT-1) +
     &                    (CSTDM(1, J)*DT)

 100  CONTINUE

*     UPDATE THE TIME-LEVEL.

      NLEVEL = TEND

      END

*************************************************************
*                    SUBROUTINE CSINP1                      *
*************************************************************
*                                                           *
*  PURPOSE  - THIS SUBROUTINE IS USED TO ESTIMATE THE REDUCED *
*             INTERSTITIUM SOLUTE CONCENTRATIONS AT THE N+1 TIME *
*             LEVEL.                                        *
*                                                           *
*  USAGE  - CALL CSINP1(PDTM, GAMA, CRM2TV, CRM1TV,         *
*                       CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM,  *
*                       CIM1TM, CITM, CIP1TM, CIP2TM, COTV, C1TV, *
*                       C2TV)                               *
*                                                           *
*  ARGUMENTS AND VARIABLES                                  *
*                                                           *
*               PDTM - VECTOR OF WATER PRODUCTION-DEPLETION TERM. *
*               GAMA - COEFFICIENT USED IN CALCULATION OF   *
*                      INTERSTITIUM CONCENTRATIONS (SEE SUBROUTINE *
*                      NLCOEF FOR DETAILS, DIMENSIONLESS).  *
*  CRM2TV, CRM1TV, CBTV, CMM1TM, CMTM, CMP1TM, CIM2TM, CIM1TM, *
*  CITM, CIP1TM, CIP2TM, COTV, C1TV, C2TV                   *
*                    - SCALARS AND VECTORS OF NON-LINEAR    *
*                      COEFFICIENTS OF THE FINITE DIFFERENCE *
*                      EQUATIONS.                           *
*   AV, BV, CV, DV, - VECTORS CONTAINING THE VALUES OF THE  *
*   EV, FV            DIAGONAL ELEMENTS OF THE PENTADIAGONAL *
*                      MATRIX OF THE SYSTEM OF LINEAR EQUATIONS *
*                      TO BE SOLVED (SEE SUBROUTINE PENTAG FOR *
*                      DETAILS, DIMENSIONLESS).             *
*             GRPCNT - SPACE GRID POINT COUNTER.            *
*             GRPTIX - SPACE GRID POINT POSITION INDEX ON THE *
*                      EXTENDED SPACE GRID.                 *
*       MATI1, MATI2 - MATRIX COLUMN POSITION INDICES.      *
*        FIRST, LAST - INDICES OF THE FIRST AND LAST EQUATIONS OF *
*                      THE SYSTEM TO BE SOLVED.             *
*                 VV - SOLUTION VECTOR OF SYSTEM OF LINEAR  *
*                      EQUATIONS.                           *
*************************************************************

      SUBROUTINE CSINP1(PDTM, GAMA, CRM2TV, CRM1TV,
      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS

      REAL*4  PDTM(0:NGRPTS),GAMA,
     &        CRM2TV, CRM1TV, CBTV,
     &        CMM1TM(NGRPTS-(2*(NCELLS+1))),
     &        CMTM(NGRPTS-(2*(NCELLS+1))),
     &        CMP1TM(NGRPTS-(2*(NCELLS+1))),
     &        CIM2TM(NCELLS-1), CIM1TM(NCELLS-1),
     &        CITM(NCELLS-1), CIP1TM(NCELLS-1),
     &        CIP2TM(NCELLS-1), COTV, C1TV,
     &        C2TV

*     COMMON VARIABLES

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELLS)
      COMMON /C8/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(8, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO

      REAL*4 CDIFCM, CSIM, CSCM, CELLM, NLEVEL, CAVG

      REAL*4 HSTEPV, KSTEP

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

*     ROUTINE VARIABLES

      REAL*4 AV(NGRPTS-NCELLS-1), BV(NGRPTS-NCELLS-1),
     &       CV(NGRPTS-NCELLS-1), DV(NGRPTS-NCELLS-1),
     &       EV(NGRPTS-NCELLS-1), FV(NGRPTS-NCELLS-1),
     &       VV(NGRPTS-NCELLS-1)

      INTEGER GRPCNT, GRPTIX, MATI1, MATI2, FIRST, LAST

*     FOR SUCROSE, USING INFORMATION AT THE N TIME LEVEL AND
*     ESTIMATES OF NON-LINEAR COEFFICIENTS AT THE N+1/2 TIME LEVEL,
*     SET UP VECTORS OF ELEMENTS OF PENTADIAGONAL MATRIX

*         FIRST SPACE GRID POINT OR CENTER

          AV(1) = 0.0
          BV(1) = 0.0
          CV(1) = 1.0 + C1TV
          DV(1) = - C2TV
          EV(1) = 0.0
          FV(1) = ((1.0 - C1TV) * CSIM(1, LVLCNT-2)) +
     &            (C2TV *  CSIM(2, LVLCNT-2))
     &            + (2.0 * COTV * CSIOV)

*         (R-1)-TH SPACE GRID POINT

          AV(RNUM-1) = 0.0
          BV(RNUM-1) = - CRM2TV
          CV(RNUM-1) = 1.0 + CRM1TV
          DV(RNUM-1) = 0.0
          EV(RNUM-1) = 0.0
          FV(RNUM-1) =
     &            (CRM2TV * CSIM(RNUMEX-2, LVLCNT-2)) +
     &            ((1.0 - CRM1TV) * CSIM(RNUMEX-1, LVLCNT-2))

          FV(RNUM-1) = FV(RNUM-1) + (2.0 * CBTV * CSBOV)

*         M-TH SPACE GRID POINT (INCLUDING INTERFACE POINTS)

          GRPCNT  = 3
          GRPTIX = 2
          GRPTI = 2
          MATI1 = 1
          MATI2 = 1

 20        CONTINUE

          IF (GRPCNT .LT. GRPCEL) THEN

            AV(GRPTI) = 0.0
            BV(GRPTI) = - CMM1TM(MATI1)
            CV(GRPTI) = 1.0 + CMTM(MATI1)
            DV(GRPTI) = - CMP1TM(MATI1)
            EV(GRPTI) = 0.0
            FV(GRPTI) =
     &        (CMM1TM(MATI1) * CSIM(GRPTIX-1, LVLCNT-2)) +
     &        ((1.0 - CMTM(MATI1)) * CSIM(GRPTIX, LVLCNT-2)) +
     &        (CMP1TM(MATI1) * CSIM(GRPTIX+1, LVLCNT-2))

            GRPCNT = GRPCNT + 1
            GRPTIX = GRPTIX + 1
            GRPTI = GRPTI + 1
            MATI1 = MATI1 + 1
            IF ((GRPTIX .EQ. RNUMEX-1) .OR. (CELNUM .EQ. 1)) GO TO 30
            GO TO 20

          ELSE

            AV(GRPTI) = - CIM2TM(MATI2)
            BV(GRPTI) = CIM1TM(MATI2)
            CV(GRPTI) = - CITM(MATI2)
            DV(GRPTI) = CIP1TM(MATI2)
            EV(GRPTI) = - CIP2TM(MATI2)
            FV(GRPTI) =
     &            (CIM2TM(MATI2) * CSIM(GRPTIX-2, LVLCNT-2)) -
     &            (CIM1TM(MATI2) * CSIM(GRPTIX-1, LVLCNT-2)) +
     &            (CITM(MATI2) * CSIM(GRPTIX, LVLCNT-2)) -
     &            (CIP1TM(MATI2) * CSIM(GRPTIX+2, LVLCNT-2)) +
     &            (CIP2TM(MATI2) * CSIM(GRPTIX+3, LVLCNT-2))

            GRPCNT = 2
            GRPTIX = GRPTIX + 2
            GRPTI = GRPTI + 1
          MATI2 = MATI2 + 1
          GO TO 20

        END IF

 30      CONTINUE

*       SOLVE SYSTEM OF LINEAR EQUATIONS

        FIRST = 1
        LAST = RNUM - 1

        CALL PENTAG(FIRST, LAST, AV, BV, CV, DV, EV, FV, VV)

        GRPCNT = 2
        GRPTIX = 1

        DO 40 K = 1, RNUM-1

           CSIM(GRPTIX, LVLCNT) = VV(K)

           IF (GRPCNT .LT. GRPCEL) THEN
             GRPCNT = GRPCNT + 1
             GRPTIX = GRPTIX + 1
            ELSE
             GRPCNT = 2

             CSIM(GRPTIX+1, LVLCNT) = CSIM(GRPTIX, LVLCNT)

             GRPTIX = GRPTIX + 2
           END IF

 40      CONTINUE

*       GET ESTIMATES OF THE INTERSTITIUM CONCENTRATION AT THE
*       CENTRE AND AT THE SURFACE OF THE TISSUE

          CSIM(0, LVLCNT) = CSIOV

          CSIM(RNUMEX, LVLCNT) = CSBOV

*    TESTING FOR THE SENSITIVITY

      DO 70 I = 0, RNUMEX
      IF(CSIM(I, LVLCNT) .LE. 1.0E-8) THEN
      CSIM(I, LVLCNT) = 0.0
      ELSE
      ENDIF
 70   CONTINUE

      END

**************************************************************
*                    SUBROUTINE PENTAG                        *
**************************************************************
*                                                             *
*  PURPOSE  - THIS SUBROUTINE IS USED TO SOLVE A SYSTEM OF LINEAR *
*             SIMULTANEOUS EQUATIONS ( A X = B ) HAVING A      *
*             PENTADIAGONAL COEFFICIENT BAND MATRIX ( A )      *
*                                                             *
*  USAGE  - CALL PENTAG(FIRST, LAST, AV, BV, CV, DV, EV, FV, VV) *
*                                                             *
*  ARGUMENTS AND VARIABLES                                    *
*                                                             *
*            THE EQUATIONS ARE NUMBERED FROM  FIRST  TO  LAST  *
*            AND THEIR SECOND, FIRST LOWER DIAGONAL, MAIN DIAGONAL,*
*            FIRST AND SECOND UPPER DIAGONAL COEFFICIENTS ARE  *
*            STORED IN THE ARRAYS AV, BV, CV, DV, EV RESPECTIVELY. *
*            FV IS AN ARRAY CONTAINING THE INFORMATION VECTOR B *
*            THE COMPUTED SOLUTION VECTOR X (X(FIRST), ...,    *
*            X(LAST)) IS STORED IN THE ARRAY VV                *
*                                                             *
*    DELTAV, LAMDAV, GAMAV - INTERNAL ARRAYS USED IN THE ALGORITHM *
*                                                             *
*                 MU, BETA - INTERMEDIATE VARIABLES APPEARING IN *
*                            THE CALCULATIONS                  *
*                                                             *
*  REMARKS  - TO KEEP ROUNDING ERRORS TO A MINIMUM, THE        *
*             CALCULATIONS ARE PERFORMED IN DOUBLE-PRECISION.  *
*             NOTE THAT THE VECTORS THAT ARE INPUT AND OUTPUT ARE *
*             IN SINGLE-PRECISION                              *
**************************************************************

      SUBROUTINE PENTAG(FIRST, LAST, SAV, SBV, SCV, SDV, SEV,
     &                  SFV, SVV)

       INTEGER NGRPTS, NCELLS

       PARAMETER(NGRPTS = 3500, NCELLS = 100)

*      ARGUMENTS

       REAL*4 SAV(NGRPTS-NCELLS-1), SBV(NGRPTS-NCELLS-1),
     &        SCV(NGRPTS-NCELLS-1), SDV(NGRPTS-NCELLS-1),
     &        SEV(NGRPTS-NCELLS-1), SFV(NGRPTS-NCELLS-1),
     &        SVV(NGRPTS-NCELLS-1)

       INTEGER FIRST, LAST

*      ROUTINE VARIABLES

       REAL*8 AV(NGRPTS-NCELLS-1), BV(NGRPTS-NCELLS-1),
     &        CV(NGRPTS-NCELLS-1), DV(NGRPTS-NCELLS-1),
     &        EV(NGRPTS-NCELLS-1), FV(NGRPTS-NCELLS-1),
     &        VV(NGRPTS-NCELLS-1), DELTAV(NGRPTS-NCELLS-1),
     &        LAMDAV(NGRPTS-NCELLS-1), GAMAV(NGRPTS-NCELLS-1),
     &        MU, BETA

*      CONVERT INCOMING VECTORS IN DOUBLE-PRECISION

       DO 10 K = FIRST, LAST
          AV(K) = DBLE(SAV(K))
          BV(K) = DBLE(SBV(K))
          CV(K) = DBLE(SCV(K))
          DV(K) = DBLE(SDV(K))
          EV(K) = DBLE(SEV(K))
          FV(K) = DBLE(SFV(K))
 10     CONTINUE

       DELTAV(FIRST) = DV(FIRST) / CV(FIRST)
      LAMDAV(FIRST) = EV(FIRST) / CV(FIRST)
      GAMAV(FIRST) = FV(FIRST) / CV(FIRST)

      MU = CV(FIRST+1) - (BV(FIRST+1) * DELTAV(FIRST))
      DELTAV(FIRST+1) = (DV(FIRST+1) - (BV(FIRST+1) *
     &                  LAMDAV(FIRST))) / MU
      LAMDAV(FIRST+1) = EV(FIRST+1) / MU
      GAMAV(FIRST+1) = (FV(FIRST+1) - (BV(FIRST+1) *
     &                 GAMAV(FIRST))) / MU

      DO 20 I = FIRST+2, LAST-2
         BETA = BV(I) - (AV(I) * DELTAV(I-2))
         MU = CV(I) - (BETA * DELTAV(I-1)) - (AV(I) * LAMDAV(I-2))
         DELTAV(I) = (DV(I) - (BETA * LAMDAV(I-1))) / MU
         LAMDAV(I) = EV(I) / MU
         GAMAV(I) = (FV(I) - (BETA * GAMAV(I-1)) -(AV(I) *
     &              GAMAV(I-2))) / MU
 20   CONTINUE

      BETA = BV(LAST-1) - (AV(LAST-1) * DELTAV(LAST-3))
      MU = CV(LAST-1) - (BETA * DELTAV(LAST-2)) - (AV(LAST-1) *
     &     LAMDAV(LAST-3))
      DELTAV(LAST-1) = (DV(LAST-1) - (BETA * LAMDAV(LAST-2))) / MU
      GAMAV(LAST-1) = (FV(LAST-1) - (BETA * GAMAV(LAST-2)) -
     &                (AV(LAST-1) * GAMAV(LAST-3))) / MU

      BETA = BV(LAST) - (AV(LAST) * DELTAV(LAST-2))
      MU = CV(LAST) - (BETA * DELTAV(LAST-1)) - (AV(LAST) *
     &     LAMDAV(LAST-2))
      GAMAV(LAST) = (FV(LAST) - (BETA * GAMAV(LAST-1)) - (AV(LAST) *
     &              GAMAV(LAST-2))) / MU

*     STORE SOLUTION OF SYSTEM IN VECTOR VV.

      VV(LAST) = GAMAV(LAST)
      VV(LAST-1) = GAMAV(LAST-1) - (DELTAV(LAST-1) * VV(LAST))
      DO 30 I = LAST-2, FIRST, -1
         VV(I) = GAMAV(I) - (DELTAV(I) * VV(I+1)) - (LAMDAV(I) *
     &   VV(I+2))
 30   CONTINUE

*     CONVERT SOLUTION VECTOR BACK TO SINGLE-PRECISION

      DO 40 K = FIRST, LAST
         SVV(K) = REAL(VV(K))
 40   CONTINUE

      END
*******************************************************************
*                        SUBROUTINE DCFUNC                        *
*******************************************************************
*                                                                 *
*  PURPOSE  - FROM AN EMPIRICAL MODEL (POLYNOMIAL OF DEGREE 1     *
*             DESCRIBING THE CONCENTRATION DEPENDENCE OF          *
*             THE SUCROSE PSEUDO-BINARY DIFFUSION COEFFICIENT,    *
*             THIS SUBROUTINE EVALUATES THE LOCAL VALUE OF THE    *
*             COEFFICIENT BASED ON THE LOCAL INTERSTITIUM         *
*             CONCENTRATION OF THE SOLUTE. THEN IT CORRECTS THE   *
*             ESTIMATE TO TAKE INTO ACCOUNT THE RESISTANCE OF THE *
*             INTERSTITIUM MICROSTRUCTURE                         *
*                                                                 *
*  USAGE   - CALL DCFUNC                                          *
*                                                                 *
*  ARGUMENTS AND VARIABLES                                        *
*                                                                 *
*          STARTX - GRID POINT POSITION INDEX ON THE EXTENDED     *
*                   SPACE GRID                                    *
*            MATI - CDIFCM MATRIX COLUMN INDEX                    *
*          NCOUNT - POSITION COUNTER FOR ELEMENTS OF VECTOR CSIV  *
*            CSIV - VECTOR OF CONCENTRATION VALUES TO BE USED IN  *
*                   THE EMPIRICAL RELATION, IN G CM-3             *
*           POLYN - CURRENT CALCULATED VALUE OF THE POLYNOMIAL    *
*                   (DIMENSIONLESS). THE POLYNOMIAL IS DEFINED AS *
*                   FOLLOWS (FOR SUCROSE)                         *
*                                                                 *
*           LN (D(I) / D(I) INFINITY) = A0 + A1*CS(I)             *
*                                                                 *
*           DCVAL - CURRENT VALUE OF THE LOCAL PSEUDO-BINARY      *
*                   DIFFUSION COEFFICIENT                         *
*          CDIFCM - MATRIX OF CORRECTED PSEUDO-BINARY COEFFICIENTS *
*******************************************************************

      SUBROUTINE DCFUNC

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS

*     COMMON VARIABLES

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C4/ CDIFCM(0 (NGRPTS*2)-NCELLS)
      COMMON /C5/ MWV(2)
      COMMON /C12/ CSIM(0 NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(5, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C14/ DIFCV, DEGV, POLCOM(0 1)

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO, CDIFCM,
     &       CSIM, CSCM, CELLM, NLEVEL, CAVG,
     &       DIFCV, POLCOM, PMVV, RT, PMV, PPV, MWV

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, DEGV

*     ROUTINE VARIABLES

      REAL*4 CSIV(((NGRPTS/NCELLS)*2)-1), POLYN, DCVAL

      INTEGER STARTX, MATI, NCOUNT

*     SET UP VECTOR OF LOCAL INTERSTITIUM CONCENTRATIONS.

      STARTX = RNUMEX - (CELLI * GRPCEL)
      MATI = ((GRPCEL * 2) - 1) * (CELNUM - CELLI)

      NCOUNT = 1
      K = 1

 10    CONTINUE

      CSIV(NCOUNT) = CSIM(STARTX+K, LVLCNT)

      IF (K .EQ. GRPCEL) GO TO 20

      CSIV(NCOUNT+1) = ((CSIM(STARTX+K, LVLCNT) +
     &            CSIM(STARTX+K+1, LVLCNT)) / 2.0)

      NCOUNT = NCOUNT + 2
      K = K + 1
      GO TO 10

 20    CONTINUE

      DO 30 I = 1, NCOUNT

        POLYN = POLCOM(0) + (POLCOM(1) * CSIV(I))

*       GET THE LOCAL VALUE OF THE DIFFUSION COEFFICIENT

        DCVAL = DIFCV * EXP(POLYN)

*       THE EXPERIMENTAL MEASUREMENTS OF DIFFUSION
*       COEFFICIENTS ARE MEASURED WITH RESPECT TO A FIXED
*       VOLUME FRAME OF REFERENCE AND THE EQUATIONS ARE
*       DEVELOPPED WITH RESPECT THE BARYCENTRIC VELOCITY

        DCVAL = (DCVAL * MWV(1)) / (PMVV(1) * CAVG)

*       CORRECT THE ABOVE COEFFICIENT TO TAKE INTO ACCOUNT THE
*       RESISTANCE OF THE INTERSTITIUM MICROSTRUCTURE

        CDIFCM(MATI) = CELLM(9, CELLI, LVLCNT) * DCVAL

        MATI = MATI + 1

 30    CONTINUE

      END

******************************************************************
*                          SUBROUTINE FLUXM                      *
******************************************************************
*                                                                *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE LOCAL WATER          *
*             TRANSMEMBRANE FROM A THERMODYNAMICAL POINT OF VIEW *
*             GIVEN AN INTRACELLULAR HYDROSTATIC PRESSURE AND A  *
*             COMPLETE COMPOSITION OF THE INTRACELLULAR          *
*             COMPARTMENT. SINCE FOR POTATO MATERIAL, THERE ARE  *
*             TWO IMPORTANT PHASES IN THE CELLULAR VOLUME        *
*             I. E. THE VACUOLE WHICH IS AN AQUEOUS SOLUTION OF  *
*             SMALL SOLUTES AND THE CYTOPLASM WHICH COMPRISES    *
*             PROTEINS AND STARCH. ASSUMING THAT BOTH PHASES     *
*             ARE IN EQUILIBRIUM, THE CHEMICAL POTENTIAL OF THE  *
*             CELLULAR VOLUME IS OBTAINED BY EITHER PHASE.       *
*             SINCE SUCROSE PENETRATES THE EXTRACELLULAR         *
*             MEDIUM, THE CHEMICAL POTENTIAL IS EQUAL TO THE     *
*             OSMOTIC POTENTIAL.                                 *
*                                                                *
*  USAGE   - CALL FLUXM(FLUXMM)                                  *
*                                                                *
*  ARGUMENTS AND VARIABLES                                       *
*                                                                *
*          FLUXMM - MATRIX OF TRANSMEMBRANE FLUXES, IN G CM-2 SEC-1*
*          FORCEV - VECTOR OF THERMODYNAMIC FORCE                *
*                   DIFFERENCE GRADIENTS.                        *
*             SUM - SUMMATION VARIABLE.                          *
*           DTERM - TERM RELATED TO THE DIFFERENCE IN CHEMICAL   *
*                   POTENTIAL DUE TO THE OSMOTIC POTENTIAL OR    *
*                   DUE TO THE MATRIC POTENTIAL INSIDE THE       *
*                   CELLULAR VOLUME AND THE OSMOTIC POTENTIAL    *
*                   IN THE EXTRACELLULAR VOLUME.                 *
*           PTERM - TERM RELATED TO HYDROSTATIC PRESSURE         *
*                   DIFFERENCE BETWEEN THE EXTRACELLULAR         *
*                   CONDITIONS AND INTRACELLULAR CONDITIONS.     *
*          T1, T2 - INTERMEDIATE VARIABLES USED IN CALCULATIONS  *
*                                                                *
*  REMARKS  -  THIS SUBROUTINE USES A ZERO FINDING FUNCTION,     *
*              (ZREAL2) IN ORDER TO ESTIMATE THE COMPLETE        *
*              COMPOSITION OF THE INTRACELLULAR VOLUME           *
*              (SEE IMSL LIBRARY FOR DETAILS).                   *
*                                                                *
*  N.B. PLEASE NOTE THAT THE WATER ACTIVITY IN THE CELLULAR      *
*       VOLUME IS EITHER CALCULATED FROM THE VACUOLAR OR THE     *
*       CYTOPLASTIC CONDITIONS SINCE WE ASSUME THAT BOTH PHASES  *
*       ARE IN EQUILIBRIUM INTANEOUSTLY.                         *
******************************************************************

      SUBROUTINE FLUXM(FLUXMM)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 FLUXMM(0:NGRPTS)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C6/ MWV(2)
      COMMON /C7/ EMODCO(2), WRESF, PCO
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C18/ XT,XST,XP,XV
      COMMON /C19/ AWVI(NCELLS),AWO
      REAL*4 SPVFO,WVFO,VOIDFO,VCO,VIO,VTO,AIO,ACMO,ACPO,
     &       LCO,RIO,RCO,RBO, STORT

*     ROUTINE VARIABLES

      REAL*4 PI

      DATA PI/3.14159/

      REAL*4 FORCEV

      REAL*4 PMVV, RT, PMV, PPV,
     &       EMODCO, WRESF, PCO, CSIM, CSCM, CELLM, NLEVEL,
     &       CAVG, AWVI

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO, MWV

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

      REAL*4 T1, T2, PTERM, OTERM, TPTERM

      REAL*4 XS, XW, GW, AWO, MS, LMW, CRIT

      INTEGER NSIG, N, ITMAX, IER
      REAL*4 B, C, F, EPS, EPS2, ETA
      REAL*4 XT, XST, XP, XV, AWI

      EXTERNAL F

*     CALCULATION OF THE LOCAL THERMODYNAMIC FORCE ACROSS
*     THE CELL MEMBRANE.

*     SET FORCEV TO 0.
          FORCEV = 0.0

*     SINCE THE CONCENTRATION AT THE SURFACE IS FIXED,
*     THE FLUX OF WATER THROUGH THE MEMBRANE IS ZERO
*     AT ANY TIME AT THIS PARTICULAR POINT BECAUSE OF THE
*     NATURE OF THE CONDITION.

          IF(GRPTI .EQ. RNUMEX) THEN
          FLUXMM(RNUMEX) = 0.0
          ELSE

*      A.  EXTRACELLULAR CONDITIONS

*          1. OSMOTIC POTENTIAL

              XS = (CSIM(GRPTI, LVLCNT) / MWV(2))
     &        / ((CSIM(GRPTI, LVLCNT) / MWV(2))
     &        + ((CAVG - CSIM(GRPTI, LVLCNT)) / MWV(1)))

              XW = (1.0 - XS)

              GW = EXP(-(XS * XS) * (3.36 + (80.4 * XS)
     &                -  (823.6 * XS * XS)))

              AWO = GW * XW

*      CORRECTION FOR THE TEMPERATURE (40 DEG. C)

              MS = XS / (XW * 1000.0)

              AWO = AWO * EXP(0.0004878 * MS*MS)

*      B.  INTRACELLULAR CONDITIONS

*          1. TERM RELATED TO HYDROSTATIC PRESSURE GRADIENT

              T1=PCO
              T2 = EMODCO(2) / EMODCO(1)
              PTERM = ((T2 + T1) * ((CELLM(1, CELLI, LVLCNT)/ VCO)
     &                **EMODCO(1)))- T2

              IF (PTERM .GT. 0.0) STAGEV(CELLI) = 1

              IF (PTERM .LE. 0.0) PTERM = 0.0

              IF ((PTERM .EQ. 0.0) .AND. (STAGEV(CELLI) .EQ. 1))
     &             STAGEV(CELLI) = 2

              CRIT = CELLM(1, CELLI, LVLCNT) / VCO

              IF(CRIT .LE. 0.3) THEN
                   STAGEV(CELLI) = 3
              ELSE
              ENDIF

*          2. TERM RELATED TO THE OSMOTIC POTENTIAL USING THE
*             VACUOLAR CONDITIONS.

*      IN ORDER TO BE ABLE TO ESTIMATE THE WATER ACTIVITY INSIDE
*      THE CELLULAR VOLUME (AWI), THE COMPLETE COMPOSITION WITH
*      RESPECT TO WATER IS NEEDED I.E. XV, XST, XP SINCE
*      CSCM(1, NCELLS, LVLCNT) REPRESENTS THE TOTAL WATER OF THE
*      CELLULAR VOLUME ON A DRY MATTER BASIS (XT).

*      CONSTANTS FOR HASLEY EQUATION AT 40 DEG. C.
       B=5.586E04
       C=1.848E0

* ESTIMATION OF OF THE FIRST GUESS OF AWI WITH THE HASLEY EQ.

       XT = CSCM(1, CELLI, LVLCNT)
       AWI = EXP(-B/((RT/1.0E04)*(XT**C)))

* CALL ZREAL2 SUBROUTINE TO COMPARE AWI AND AWV
* UNTIL CONVERGENCE IN ORDER TO FIND THE COMPLETE COMPOSITION.
* SETTING THE PARAMETERS USED IN ZREAL2.

       EPS=1.0E-5
       EPS2=1.0E-3
       ETA=1.0E-3
       NSIG=5
       ITMAX=100
       N=1

       CALL ZREAL2(F,EPS,EPS2,ETA,NSIG,N,AWI,ITMAX,IER)
```

```
*     THE VALUES OF AWI ARE STORED FOR FURTHER CALCULATIONS
*     IN THE SYMPLAST TRANSPORT. VALUES FOR THE COMPLETE
*     COMPOSITION ARE ALSO STORED IN THE MATRIX.

                AWVI(CELLI) = AWI
           CSCM (2, CELLI, LVLCNT) = XST
           CSCM (3, CELLI, LVLCNT) = XP
           CSCM (4, CELLI, LVLCNT) = XV

*     THE DIFFERENCE BETWEEN THE OSMOTIC POTENTIAL IN THE
*     EXTRACELLULAR VOLUME AND THE CELLULAR VOLUME.

              OTERM = RT * ALOG (AWI / AWO)

*     THE GRADIENT OF THERMODYNAMIC FORCE ACROSS THE
*     MEMBRANE IS DEFINED AS:

              FORCEV = OTERM + (PMVV(1) * PTERM)

*     SINCE THE THERMODYNAMIC FORCE IS EXPRESSED IN TERMS OF
*     CHEMICAL POTENTIAL, THE PERMEABILITY COEFFICIENT IS
*     TRANSFORMED ACCORDINGLY. THE PERMEABILITY COEFFICIENT IS
*     DEPENDENT ON THE SUCROSE CONCENTRATION OF THE
*     EXTRACELLULAR SPACE.

          PMV=4.25E-04 * EXP(-3.0 * CSIM(GRPTI,LVLCNT))

             LMW = (PMV * MWV(1)) / (RT * PMVV(1))

*     THE FLUX OF WATER ACROSS THE MEMBRANE IS THEN:

              FLUXMM(GRPTI) = LMW * FORCEV

*     CONDITION FOR THE SENSITIVITY OF THE TRANSMEMBRANE FLUX.

          IF (ABS(FLUXMM(GRPTI)) .LE. 1.0E-11) THEN
               FLUXMM(GRPTI) = 0.0
          ELSE
          ENDIF

      ENDIF

      RETURN

      END
***********************************************************************
*                          REAL FUNCTION F                            *
***********************************************************************
*                                                                     *
*  PURPOSE: THIS SUBROUTINE IS CALLED BY ZREAL2 TO PERFORM            *
*           THE ESTIMATION OF THE COMPLETE COMPOSITION  KNOWING       *
*           THE TOTAL WATER CONTENT XT.  A GUESS IS USED ON AWI,      *
*           THE COMPOSITION XST AND XP ARE ESTIMATED. XV IS           *
*           CALCULATED BY DIFFERENCE. AWV IS THEN CALCULATED AND      *
*           COMPARED WITH AWI UNTIL CONVERGENCE.                      *
*                                                                     *
*      EMPIRICAL CORRELATIONS ARE USED TO DETERMINE THE WATER         *
*      CONTENT OF STARCH (XST) AND PROTEINS (XP). THEY WERE           *
*      BY CRAPISTE AND ROTSTEIN (1982).                               *
*                                                                     *
*      FOR STARCH:                                                    *
*                                                                     *
*        RT LN AWI = RT LN (1 - EXP( -53.4759 (XST ** 2.3015)))       *
*                                                                     *
*      FOR PROTEINS:                                                  *
*                                                                     *
*        RT LN AWI = RT LN (- 0.0208 (XP ** - 1.8129))                *
*                                                                     *
*      FOR VACUOLE, ON A BINARY BASIS, CALCULATE THE AW OF EACH       *
*      COMPONENT AND USING THE ROSS(1975) EQUATION, GET THE AWV.      *
*      (CRAPISTE AND ROTSTEIN, 1982).                                 *
***********************************************************************
      REAL FUNCTION F(AWI)

      REAL*4 WKP,WKS,WS,WG,WF,WP,WST
      REAL*4 XWG,XWF,XWS,XWKP,XWKS
      REAL*4 MWV,MG,MF,MKP,MKS
      REAL*4 ALG,ALF,ALS,ALKP,ALKS
      REAL*4 AWG,AWF,AWS,AWKP,AWKS,AWV,AWI
      REAL*4 XT,XST,XP,XV

      COMMON /C6/ MWV(2)
      COMMON /C17/ WG,WF,WS,WKP,WKS,WST,WP,MG,MF,MKP,MKS
      COMMON /C18/ XT,XST,XP,XV

*     CALCULATION OF XST, THE WATER CONTENT OF THE STARCH.

      XST=(-(ALOG(1.0-AWI))/53.4759)**(1.0/2.3015)

*     CALCULATION OF XP, THE WATER CONTENT OF THE PROTEINS.

      XP=(-(ALOG(AWI))/0.0208)**(-1.0/1.8129)

*     CALCULATION OF XV, THE WATER CONTENT OF THE VACUOLE
*     BY DIFFERENCE

      XV= XT - (WST*XST) - (WP*XP)

*     CALCULATION OF ALP.

      ALG=MWV(1)/MG
      ALF=MWV(1)/MF
      ALS=MWV(1)/MWV(2)
      ALKP=MWV(1)/MKP
      ALKS=MWV(1)/MKS

*     CALCULATION OF MOLE FRACTION OF EACH COMPONENT OF THE VACUOLE.

      XWG = XV / (XV + (WG * ALG))
      XWF = XV / (XV + (WF * ALF))
      XWS = XV / (XV + (WS * ALS))
      XWKP= XV / (XV + (WKP * ALKP))
      XWKS= XV / (XV + (WKS * ALKS))

*     ON A BINAY BASIS: WATER-I-TH COMPONENT.

      AWG = (10.**(-0.858 * ((1-XWG)**2.))) * XWG
      AWF = (10.**(-0.858 * ((1-XWF)**2.))) * XWF
      AWS = (10.**(-2.772 * ((1-XWS)**2.))) * XWS
      AWKP= (10.**(-0.718 * ((1-XWKP)**1.))) * XWKP
      AWKS= (10.**(-0.487 * ((1-XWKS)**1.))) * XWKS

*     THE PRODUCT OF THE AW OF EACH COMPONENT GIVES AWV.

      AWV = AWG * AWF * AWS * AWKP * AWKS

*     COMPARISON OF THE ESTIMATE OF AWI TO THE CALCULATED VALUE
*     AWV UNTIL CONVERGENCE.

      F=AWV-AWI

      RETURN

      END

**********************************************************************
*                         SUBROUTINE FLUXP                           *
**********************************************************************
*                                                                    *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE J-TH CELL MODIFIED       *
*             PLASMODESMAL FLUXES (J, (J-1)-TH CELL INTERFACE)       *
*             FOR GIVEN J, (J-1)-TH CELL SOLUTE CONCENTRATIONS       *
*             IN ORDER TO CALCULATE THE CHEMICAL POTENTIAL OF        *
*             BOTH CELL AND HYDROSTATIC PRESSURES.                   *
*                                                                    *
*  USAGE   - CALL FLUXP(FLUXPM)                                      *
*                                                                    *
*  ARGUMENTS AND VARIABLES                                           *
*                                                                    *
*          FLUXPM - MATRIX OF PLASMODESMAL FLUXES, IN G CM-3 SEC-1   *
*          FORCEV - VECTOR OF THERMODYNAMIC FORCE                    *
*                   DIFFERENCE GRADIENTS.                            *
*             SUM - SUMMATION VARIABLE                               *
*           CTERM - TERM RELATED TO CONCENTRATION GRADIENT(S) IN     *
*                   CHEMICAL POTENTIAL GRADIENT, IN G CM-3.          *
*          T1, T2 - INTERMEDIATE VARIABLES USED IN CALCULATIONS.     *
*        PJ, PJM1 - HYDROSTATIC PRESSURE IN THE J-TH AND (J-1)-TH    *
*                   CELL RESPECTIVELY, IN G CM-3.                    *
*           PTERM - TERM RELATED TO HYDROSTATIC PRESSURE GRADIENT    *
*                   IN CHEMICAL POTENTIAL GRADIENT, IN G CM-3.       *
**********************************************************************

      SUBROUTINE FLUXP(FLUXPM)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 FLUXPM(NCELLS, 2)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO,
     &            ACMO, ACPO, LCO, RIO, RCO, RBO,GTORT
      COMMON /C6/ MWV(2)
      COMMON /C7/ EMODCO(2), WRESF, PCO
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(5, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C18/ AWVI(NCELLS),AWO

*     COMMON VARIABLES.

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

      REAL*4 PMVV, RT, PMV, PPV,
     &       EMODCO, WRESF, PCO, CSIM, CSCM, CELLM, NLEVEL, CAVG,
     &       AWVI, AWO

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO, MWV

      REAL*4 SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO,
     &       ACMO, ACPO, LCO, RIO, RCO, RBO,GTORT

*     ROUTINE VARIABLES.

      REAL*4 FORCEV

      REAL*4 T1, T2, PJ, PJM1, PTERM, OTERM, LPW

*     SET TO FORCEV = 0.

         FORCEV = 0.0

      IF ((NLEVEL .LE. 0.0) .AND. (CELLI .EQ. 1)) THEN
          FLUXPM(CELLI, 1) = 0.0
      ELSE IF (CELLI .EQ. CELNUM+1) THEN
             FLUXPM(CELLI-1, 2) = 0.0
          ELSE

*      ESTIMATION OF THE DIFFERENCE GRADIENTS OF THE
*      THERMODYNAMIC FORCES ACROSS THE INTERFACE.

*      1. TERM RELATED TO HYDROSTATIC PRESSURE GRADIENT.

          IF (STAGEV(CELLI) .GE. 2) THEN

             PJ = 0.0

          ELSE

          T1 = PCO
          T2 = EMODCO(2) /  EMODCO(1)
          PJ = ((T2 + T1) * ((CELLM(1, CELLI, LVLCNT) / VCO)
     &           **EMODCO(1)))- T2

          END IF

          IF ((STAGEV(CELLI-1) .GE. 2) .OR. (CELLI-1 .EQ. 0)) THEN
             PJM1 = 0.0
          ELSE
```

```
            T1 = PCO
            T2 = EMODCO(2) /  EMODCO(1)
            PJM1 = ((T2 + T1) * ((CELLM(1,CELLI-1, LVLCNT) / VCO)
     &              **EMODCO(1)))- T2

         END IF

         PTERM = PJ - PJM1

*     2. TERM RELATED TO OSMOTIC GRADIENTS OF BOTH TERMS.

*     CONDITION FOR THE FIRST CELL.

        IF(CELLI .EQ. 1) THEN
        DTERM = RT * ALOG (AWVI(CELLI) / AWO)
        ELSE
        DTERM = RT * ALOG (AWVI(CELLI) / AWVI(CELLI-1))
        ENDIF

        FORCEV = (PMVV(1) * PTERM) + DTERM

*      TRANSFORMATION OF THE MEMBRANE PERMEABILITY
*      IN PROPER UNITS.

        LPW = (PPV * MWV(1)) / (RT * PMVV(1))

*      EVALUATE PLASMODESMAL FLUXES.

        FLUXPM(CELLI, 1) = LPW * FORCEV

*      THE J, (J+1)-TH CELL INTERFACE FLUXES OF THE
*      PRECEDING CELL IN THE SEQUENCE ((J-1)-TH CELL) ARE
*      SIMPLY THE NEGATIVE VALUES OF THE J, (J-1)-TH CELL
*      INTERFACE FLUXES OF THE CURRENT J-TH CELL.

            IF (CELLI .NE. 1) THEN

                FLUXPM(CELLI-1, 2) = - FLUXPM(CELLI, 1)

            END IF

      END IF

      END

******************************************************************
*                        SUBROUTINE VELOCT                       *
******************************************************************
*                                                                *
*  PURPOSE  - THIS SUBROUTINE IS USED TO EVALUATE THE LOCAL      *
*             MASS AVERAGE VELOCITIES FROM ESTIMATES             *
*             OF THE LOCAL VELOCITY GRADIENTS.                   *
*                                                                *
*  USAGE   - CALL VELOCT(VELGRV, VELV)                           *
*                                                                *
*  ARGUMENTS AND VARIABLES                                       *
*                                                                *
*           VELGRV - VECTOR OF MASS AVERAGE VELOCITY GRADIENTS.  *
*             VELV - VECTOR OF MASS AVERAGE VELOCITIES.          *
*           STARTX - GRID POINT POSITION INDEX ON THE EXTENDED   *
*                    SPACE GRID.                                 *
*              SUM - SUMMATION VARIABLE.                         *
* X, Y, NX, C, IC - VARIABLES USED IN SUBROUTINES IOMSCU AND     *
* A, B, O, IER       DCSODU. SEE IMSL LIBRARY ROUTINE DESCRIPTIONS *
*                    FOR DETAILS.                                *
*                                                                *
*  REMARKS  - THIS SUBROUTINE USES A QUASI-CUBIC HERMITE         *
*             INTERPOLATION PROCEDURE TO GENERATE SPLINE         *
*             COEFFICIENTS THAT ARE USED, THROUGH A CUBIC SPLINE *
*             QUADRATURE ALGORITHM, TO ESTIMATE THE INTEGRAL OF  *
*             THE LOCAL VOLUME AVERAGE VELOCITY GRADIENTS AT EACH *
*             GRID POINT ON A CELL BY CELL BASIS (SEE IMSL LIBRARY *
*             FOR DETAILS ON ROUTINE IOMSCU AND DCSODU).         *
******************************************************************

      SUBROUTINE VELOCT(VELGRV, VELV)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 VELGRV(0:NGRPTS), VELV(0:NGRPTS)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C9/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(8, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI

      REAL*4 HSTEPV, KSTEP, CSIM, CSCM, CELLM, NLEVEL, CAVG

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

*     ROUTINE VARIABLES.

      REAL*4 SUM, X(NGRPTS/NCELLS), Y(NGRPTS/NCELLS),
     &       C(NGRPTS/NCELLS, 3), A, B, O

      INTEGER STARTX, NX, IC, IER

      DO 10 J = CELNUM, 1, -1

         CELLI = J
         STARTX = RNUMEX - (CELLI * GRPCEL)

*        THE VELOCITY AT EACH EXTENDED SPACE GRID POINT IS EVALUATED
*        USING THE CUBIC SPLINE INTEGRATION ROUTINE.

*        USING QUASI-HERMITE SPLINE, GENERATE MATRIX OF SPLINE
*        COEFFICIENTS (FOR J-TH CELL).

         SUM = 0.0
         DO 20 K = CELNUM, CELLI+1, -1
```

```
            SUM = SUM + CELLM(7, K, LVLCNT)
 20        CONTINUE

          X(1) = SUM
          Y(1) = VELGRV(STARTX+1)
          DO 30 K = 1, GRPCEL-1
             X(K+1) = SUM + (K * HSTEPV(CELLI))
             Y(K+1) = VELGRV(STARTX+1+K)
 30       CONTINUE

          NX = GRPCEL
          IC = NGRPTS/NCELLS

          CALL IQHSCU(X, Y, NX, C, IC, IER)

*         INTEGRATE THE SPLINE OVER THE REQUIRED INTERVAL.

          A = X(1)

          DO 40 K = 1, GRPCEL-1
             B = X(K+1)
             CALL DCSQDU(X, Y, NX, C, IC, A, B, Q, IER)
             VELV(STARTX+1+K) =  Q + VELV(STARTX+1)
 40        CONTINUE

*      FOR THE CONDITIONS AT THE INTERFACE SEPARATING
*      TWO ADJOINING CELLS.

          IF (CELLI .EQ. 1) GO TO 80
          VELV(STARTX+1+GRPCEL) =
     &     (CELLM(8, CELLI, LVLCNT) / CELLM(8, CELLI-1, LVLCNT)) *
     &     VELV(STARTX+GRPCEL)

 10     CONTINUE

 80     CONTINUE

       RETURN

       END

*********************************************************************
*                        SUBROUTINE FLUXA                           *
*********************************************************************
*                                                                   *
*  PURPOSE   - THIS SUBROUTINE EVALUATES THE LOCAL VALUES OF THE    *
*              REDUCED APOPLASTIC FLUXES. IT ESTIMATES THE          *
*              RELATIVE CONTRIBUTION OF DIFFUSION AND CONVECTION    *
*              IN THE OVERALL MASS TRANSPORT PHENOMENA.             *
*                                                                   *
*  USAGE   - CALL FLUXA(VELV, FLUXAM)                               *
*                                                                   *
*  ARGUMENTS AND VARIABLES.                                         *
*                                                                   *
*             VELV - VECTOR OF MASS AVERAGE VELOCITIES.             *
*           FLUXAM - MATRIX OF LOCAL VALUES OF APOPLASTIC FLUXES    *
*           STARTX - GRID POINT POSITION INDEX ON THE EXTENDED      *
*                    SPACE GRID.                                    *
*             MATI - MATRIX COLUMN INDEX.                           *
*              SUM - SUMMATION VARIABLE.                            *
* X, Y, NX, C,     - VARIABLES USED IN SUBROUTINES IQHSCU AND       *
* IC, U, DS, M1,     DCSEVU. SEE IMSL LIBRARY ROUTINE DESCRIPTIONS  *
* DDS, M2, IER       FOR DETAILS.                                   *
*                                                                   *
*  REMARKS   - THIS SUBROUTINE USES A QUASI-CUBIC HERMITE           *
*              INTERPOLATION PROCEDURE TO GENERATE SPLINE           *
*              COEFFICIENTS THAT ARE USED, THROUGH A CUBIC SPLINE   *
*              DERIVATIVE EVALUATOR, TO ESTIMATE THE SOLUTE         *
*              CONCENTRATION GRADIENTS AT EACH GRID POINT IN THE    *
*              INTERSTITIUM (SEE IMSL LIBRARY FOR DETAILS ON        *
*              ROUTINE IQHSCU AND DCSEVU).                          *
*********************************************************************

        SUBROUTINE FLUXA(VELV, FLUXAM)

        INTEGER  NGRPTS, NCELLS

        PARAMETER(NGRPTS = 3500, NCELLS = 100)

*       ARGUMENTS.

        REAL*4 VELV(0:NGRPTS), FLUXAM(2, 0:NGRPTS, 3)

*       COMMON VARIABLES.

        COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
        COMMON /C2/ PMVV(2), RT, PMV, PPV
        COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELLS)
        COMMON /C9/ HSTEPV(NCELLS), KSTEP
        COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &               CELLM(8, NCELLS, 3),
     &               STAGEV(NCELLS), CAVG
        COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI

        REAL*4 PMVV, RT, PMV, PPV, CDIFCM, HSTEPV, KSTEP, CSIM, CSCM,
     &         CELLM, NLEVEL

        INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &          COLNUM, STAGEV, LVLCNT, GRPTI, CELLI

*       ROUTINE VARIABLES.

        REAL*4 SUM, X(NGRPTS/NCELLS), U(NGRPTS/NCELLS),
     &         Y(NGRPTS/NCELLS), C(NGRPTS/NCELLS, 3),
     &         DS(NGRPTS/NCELLS), DDS(1), CAVG

        INTEGER STARTX, MATI, NX, IC, IER, M1, M2

        DO 10 J = 1, CELNUM

           CELLI = J
           STARTX = RNUMEX - (CELLI * GRPCEL)
           MATI = ((GRPCEL * 2) - 1) * (CELNUM - CELLI)

*          THE INTERSTITIUM CONCENTRATION GRADIENTS FOR SUCROSE
*          AND THE J-TH CELL ARE EVALUATED USING CUBIC SPLINE
*          DERIVATIVE EVALUATOR.

*          USING QUASI-HERMITE SPLINE, GENERATE MATRIX OF SPLINE
*          COEFFICIENTS (FOR J-TH CELL).
```

```
      SUM = 0.0
      DO 20 K = CELNUM, CELLI+1, -1
         SUM = SUM + CELLM(7, K, LVLCNT)
 20       CONTINUE

      X(1) = SUM
      U(1) = X(1)
      Y(1) = CSIM(STARTX+1, LVLCNT)
      DO 30 K = 1, GRPCEL-1
         X(K+1) = SUM + (K * HSTEPV(CELLI))
         U(K+1) = X(K+1)
         Y(K+1) = CSIM(STARTX+1+K, LVLCNT)
 30       CONTINUE

      NX = GRPCEL
      IC = NGRPTS / NCELLS

      CALL IOMSCU(X, Y, NX, C, IC, IER)

*     EVALUATE LOCAL CONCENTRATION GRADIENTS

      M1 = GRPCEL
      M2 = 0

      CALL DCSEVU(X, Y, NX, C, IC, U, DS, M1, DDS, M2, IER)

*     EVALUTE LOCAL APOPLASTIC FLUXES.

      DO 40 K = 1, GRPCEL

*        DIFFUSIVE FLUX.
         FLUXAM(2,STARTX+K, 1) = - (CDIFCM(MATI) * DS(K))

*        CONVECTIVE FLUX.
         FLUXAM(2,STARTX+K, 2) = CSIM(STARTX+K, LVLCNT) *
     &                           VELV(STARTX+K)

*        NET FLUX.
         FLUXAM(2,STARTX+K, 3) = FLUXAM(2,STARTX+K, 1) +
     &                           FLUXAM(2,STARTX+K, 2)

         MATI = MATI + 2

 40       CONTINUE

 10    CONTINUE

*     ESTIMATE WATER NET FLUX AT EACH EXTENDED SPACE GRID POINT.

      DO 50 J = 0, RNUMEX

         FLUXAM(1, J, 3) = (VELV(J) * CAVG) - FLUXAM(2, J, 3)

 50    CONTINUE

      DO 70 I = 0, RNUMEX
           IF(ABS(FLUXAM(2, I, 1)) .LE. 1.0E-12) THEN
                 FLUXAM(2, I, 1) = 0.0
           ELSE IF(ABS(FLUXAM(2, I, 2)) .LE. 1.0E-12) THEN
                 FLUXAM(2, I, 2) = 0.0
           ELSE IF (ABS(FLUXAM(2, I, 3)) .LE. 1.0E-12) THEN
                 FLUXAM(2, I, 3) = 0.0
           ELSE IF (ABS(FLUXAM(1, I, 3)) .LE. 1.0E-12) THEN
                 FLUXAM(1, I, 3) = 0.0
           ELSE
           ENDIF
 70   CONTINUE

      END

*******************************************************************
*                      SUBROUTINE CVFUNC                          *
*******************************************************************
*                                                                 *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE CURRENT J-TH CELL     *
*             CELLULAR, INTERSTITIUM AND TOTAL UNIT               *
*             VOLUME TIME DERIVATIVES.                            *
*                                                                 *
*  USAGE  - CALL CVFUNC(FLUXMM, FLUXPM, CVTDM)                    *
*                                                                 *
*  ARGUMENTS AND VARIABLES                                        *
*                                                                 *
*           FLUXMM - MATRIX OF TRANSMEMBRANE FLUXES, IN G CM-3 SEC-1*
*           FLUXPM - MATRIX OF PLASMODESMAL FLUXES, IN G CM-3 SEC-1 *
*            CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES, *
*                    IN CM3 SEC-1.                                *
*           STARTX - GRID POINT POSITION INDEX ON THE EXTENDED    *
*                    SPACE GRID.                                  *
*        SUMV, SUM - SUMMATION VARIABLES.                         *
* X, Y, NX, C, IC - VARIABLES USED IN SUBROUTINES IOMSCU AND      *
* A, B, Q, IER       DCSODU. SEE IMSL LIBRARY ROUTINE DESCRIPTIONS *
*                    FOR DETAILS.                                 *
*  SUMPM1, SUMPP1 - SUMMATION VARIABLES.                          *
*                                                                 *
*  REMARKS  - THIS SUBROUTINE USES A QUASI-CUBIC HERMITE          *
*             INTERPOLATION PROCEDURE TO GENERATE SPLINE          *
*             COEFFICIENTS THAT ARE USED, THROUGH A CUBIC SPLINE  *
*             QUADRATURE ALGORITHM, TO ESTIMATE THE INTEGRAL OF   *
*             THE LOCAL TRANSMEMBRANE VOLUME FLUXES OVER THE      *
*             LENGTH OF THE CELL (SEE IMSL LIBRARY                *
*             FOR DETAILS ON ROUTINE IOMSCU AND DCSODU).          *
*******************************************************************

      SUBROUTINE CVFUNC(FLUXMM, FLUXPM, CVTDM)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 FLUXMM(0:NGRPTS), FLUXPM(NCELLS, 2),
     &       CVTDM(3, NCELLS)

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C2/ PMVV(2), RT, PMV, PPV
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &              ACPO, LCO, RIO, RCO, RBO, STORT
      COMMON /C8/ MWV(2)
      COMMON /C9/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &               CELLM(8, NCELLS, 3),
     &               STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C15/ COMPFV(3)
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 PMVV, RT, PMV, PPV,
     &       SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO,
     &       ACMO, ACPO, LCO, RIO, RCO, RBO, STORT,
     &       HSTEPV, KSTEP, CSIM, CSCM, CELLM,
     &       NLEVEL, COMPFV, CAVG, MWV, PPINT

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, TM, PINT

*     ROUTINE VARIABLES.

      REAL* 4 PI

      DATA PI/3.14159/

      REAL*4 SUM, SUMV(NGRPTS/NCELLS), X(NGRPTS/NCELLS),
     &       Y(NGRPTS/NCELLS), C(NGRPTS/NCELLS, 3), A, B, Q, SUMPM1,
     &       SUMPP1

      INTEGER STARTX, NX, IC, IER, FPLASM, FAREA

*     EVALUATE LOCAL TRANSMEMBRANE WATER VOLUME FLUXES.

      STARTX = RNUMEX - (CELLI * GRPCEL)
      DO 10 K = 1, GRPCEL
         SUMV(K) = FLUXMM(STARTX+K) * PMVV(1) / MWV(1)
 10    CONTINUE

*     USING QUASI-HERMITE SPLINE, GENERATE MATRIX OF SPLINE
*     COEFFICIENTS.

      SUM = 0.0
      DO 30 K = CELNUM, CELLI+1, -1
         SUM = SUM + CELLM(7, K, LVLCNT)
 30    CONTINUE

      X(1) = SUM
      Y(1) = SUMV(1)
      DO 40 K = 1, GRPCEL-1
         X(K+1) = SUM + ( K * HSTEPV(CELLI))
         Y(K+1) = SUMV(K+1)
 40    CONTINUE

      NX = GRPCEL
      IC = NGRPTS / NCELLS

      CALL IQHSCU(X, Y, NX, C, IC, IER)

*     INTEGRATE THE SPLINE OVER THE REQUIRED INTERVAL.

      A = X(1)
      B = X(GRPCEL)

      CALL DCSQDU(X, Y, NX, C, IC, A, B, Q, IER)

*     ESTIMATE THE CELLULAR VOLUME TIME DERIVATIVE.

*     FLAG TO INDICATE IF THE SYMPLAST TRANSPORT IS PRESENT.

      IF(FPLASM .EQ. 1) THEN

         SUMPM1 = FLUXPM(CELLI, 1) * PMVV(1) / MWV(1)
         SUMPP1 = FLUXPM(CELLI, 2) * PMVV(1) / MWV(1)
      ELSE

         SUMPM1 = 0.0
         SUMPP1 = 0.0

      ENDIF

      CVTDM(1, CELLI) = -(2.0 * PI * CELLM(5, CELLI, LVLCNT) * Q) -
     &          (ACPO * SUMPM1) - (ACPO * SUMPP1)

*     ESTIMATE INTERSTITIUM AND TOTAL UNIT VOLUME TIME DERIVATIVES.

      CVTDM(2, CELLI) = COMPFV(STAGEV(CELLI))* CVTDM(1, CELLI)

      CVTDM(3, CELLI) = (1.0 + COMPFV(STAGEV(CELLI)))*
     &                    CVTDM(1, CELLI)

      END

*******************************************************************
*                        SUBROUTINE GPFUNC                        *
*******************************************************************
*                                                                 *
*  PURPOSE  - THIS SUBROUTINE EVALUATES, FOR EACH CELL, THE       *
*             CURRENT TIME DERIVATIVES OF THE REDUCED CELL LENGTH, *
*             CELL INTERSTITIUM, CELLULAR AND BUFFER RADII, OF THE *
*             APPARENT INTERSTITIUM RESISTANCE FACTOR AND OF THE  *
*             APOPLASTIC TRANSFER AREA.                           *
*                                                                 *
*  USAGE  - CALL GPFUNC(CVTDM, GPTDM)                             *
*                                                                 *
*  ARGUMENTS AND VARIABLES                                        *
*                                                                 *
*           CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES.  *
*           GPTDM - MATRIX OF UNIT CELL GEOMETRICAL MENSURATIONS  *
*                   TIME DERIVATIVES.                             *
*              PI - PI CONSTANT (DIMENSIONLESS).                  *
* T1, T2, T3, T4, - INTERMEDIATE VARIABLES USED IN CALCULATIONS.  *
*******************************************************************

      SUBROUTINE GPFUNC(CVTDM, GPTDM)

      INTEGER NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.
```

```
      REAL*4 CVTDM(3, NCELLS), GPTDM(6, NCELLS)

*     COMMON VARIABLES.

      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C7/ EMODCO(2), WRESF, PCO
      COMMON /C12/ CSIM(O:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C1[illegible]/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO, ACPO,
     &       LCO, RIO, RCO, RBO, EMODCO, WRESF, PCO, CSIM, CSCM,
     &       CELLM, NLEVEL, CAVG, GTORT, PPINT

      INTEGER STAGEV, LVLCNT, GRPTI, CELLI, FPLASM, FAREA, TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 PI, T1, T2, T3, T4
      DATA PI/3.14159/

*     EVALUATE CELL LENGTH TIME DERIVATIVE.

      GPTDM(1, CELLI) =
     &    (SQRT(GTORT)*((6.0/PI)**(1.0/3.0))*CVTDM(3,CELLI))
     &      /((CELLM(3,CELLI,LVLCNT)**(2.0/3.0))*3.0)

*     EVALUATE INTERSTITIUM CYLINDER RADIUS TIME DERIVATIVE.

      GPTDM(2, CELLI) =
     & (- ACMO * GPTDM(1, CELLI))
     &  / (2.0 * PI * CELLM(7, CELLI, LVLCNT)
     &    * CELLM(7, CELLI, LVLCNT))

*     EVALUATE CELLULAR CYLINDER RADIUS TIME DERIVATIVE.

      T1 = 1.0 / (2.0 * PI * CELLM( 4, CELLI, LVLCNT))
      T2 = CVTDM(1, CELLI) / CELLM(7, CELLI, LVLCNT)
      T3 = (CELLM(1, CELLI, LVLCNT) * GPTDM(1, CELLI))
     &     / (CELLM(7, CELLI, LVLCNT) * CELLM(7, CELLI, LVLCNT))
      T4 = (CELLM(5, CELLI, LVLCNT) * GPTDM(2, CELLI))
     &     / CELLM(4, CELLI, LVLCNT)

      GPTDM(3, CELLI) = (T1 * ( T2 - T3)) + T4

*     EVALUATE BUFFER CYLINDER RADIUS TIME DERIVATIVE.

      T1 = (CELLM(5, CELLI, LVLCNT) * GPTDM(2, CELLI))
     &     / CELLM(6, CELLI, LVLCNT)
      T2 = 1.0 / (2.0 * PI * CELLM(6, CELLI, LVLCNT))
      T3 = CVTDM(2, CELLI) / CELLM( 7, CELLI, LVLCNT)
      T4 = (CELLM(2, CELLI, LVLCNT) * GPTDM(1, CELLI))
     &     /(CELLM(7, CELLI, LVLCNT) * CELLM(7, CELLI, LVLCNT))

      GPTDM(4, CELLI) = T1 - (T2 * (T3 - T4))

*     EVALUATE TIME DERIVATIVE OF APPARENT INTERSTITIUM
*     RESISTANCE FACTOR.

      GPTDM(5, CELLI) = (1.0 - WRESF) * (WVFO * VTO) *
     &    CVTDM(2,CELLI) /
     &    (CELLM(2, CELLI, LVLCNT) * CELLM(2, CELLI, LVLCNT))

*     FINALLY, EVALUATE TIME DERIVATIVE OF APOPLASTIC TRANSFER AREA.

      T1 = 2.0 * PI * CELLM(5, CELLI, LVLCNT) * GPTDM(2, CELLI)
      T2 = 2.0 * PI * CELLM(6, CELLI, LVLCNT) * GPTDM(4, CELLI)

      GPTDM(6, CELLI) = T1 - T2

      END

*******************************************************************
*                       SUBROUTINE CCFUNC                         *
*******************************************************************
*                                                                 *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE CURRENT J-TH CELL     *
*             WATER CONCENTRATION TIME DERIVATIVES.               *
*                                                                 *
*  USAGE  - CALL CCFUNC(FLUXMM, FLUXPM, CVTDM, CSTDM)             *
*                                                                 *
*  ARGUMENTS AND VARIABLES                                        *
*                                                                 *
*           FLUXMM - MATRIX OF TRANSMEMBRANE FLUXES, IN G CM-3 SEC-1*
*           FLUXPM - MATRIX OF PLASMODESMAL FLUXES, IN G CM-3 SEC-1 *
*            CVTDM - MATRIX OF UNIT CELL VOLUME TIME DERIVATIVES  *
*                    IN CM3 SEC-1                                 *
*            CSTDM - MATRIX OF CELL WATER CONCENTRATION TIME      *
*                    DERIVATIVES IN G WATER G DRY MATTER-1 SEC-1  *
*           STARTX - GRID POINT POSITION INDEX ON THE EXTENDED    *
*                    SPACE GRID.                                  *
*              SUM - SUMMATION VARIABLE.                          *
* X, Y, NX, C, IC  - VARIABLES USED IN SUBROUTINES IOHSCU AND     *
* A, B, O, IER       DCSODU. SEE IMSL LIBRARY ROUTINE DESCRIPTIONS *
*                    FOR DETAILS.                                 *
*                                                                 *
*  REMARKS  - THIS SUBROUTINE USES A QUASI-CUBIC HERMITE          *
*             INTERPOLATION PROCEDURE TO GENERATE SPLINE          *
*             COEFFICIENTS THAT ARE USED, THROUGH A CUBIC SPLINE  *
*             QUADRATURE ALGORITHM, TO ESTIMATE THE INTEGRAL OF   *
*             THE LOCAL TRANSMEMBRANE WATER FLUX OVER THE         *
*             LENGTH OF THE CELL (SEE IMSL LIBRARY                *
*             FOR DETAILS ON ROUTINE IOHSCU AND DCSQDU).          *
*******************************************************************

      SUBROUTINE CCFUNC(FLUXMM, FLUXPM, CVTDM, CSTDM)

      INTEGER  NGRPTS, NCELLS

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 FLUXMM(O:NGRPTS), FLUXPM(NCELLS, 2),
     &       CVTDM(3, NCELLS), CSTDM(1, NCELLS)
```

```
*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C3/ CSBOV, CSIOV, XTO, XSTO, XPO, XVO
      COMMON /C6/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C7/ EMODCO(2), WRESF, PCO
      COMMON /C8/ HSTEPV(NCELLS), KSTEP
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(9, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C16/ FPLASM, FAREA, TM, PINT, PPINT
      COMMON /C20/ DDM, DW

      REAL*4 EMODCO, WRESF, PCO,
     &       HSTEPV, KSTEP, CSIM, CSCM, CELLM, NLEVEL, CAVG,
     &       DDM, DW, MDM, PPINT

      REAL*4 CSBOV, CSIOV, CDIFCM, XTO, XSTO, XPO, XVO

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, TM, PINT

*     ROUTINE VARIABLES.

      REAL*4 PI

      DATA PI/3.14159/

      REAL*4 SUM, X(NGRPTS/NCELLS), Y(NGRPTS/NCELLS),
     &       C(NGRPTS/NCELLS, 3), A, B, Q, T1, T2, T3

      REAL*4 SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &       ACPO, LCO, RCO, RIO, RBO, GTORT

      INTEGER STARTX, NX, IC, IER, FPLASM, FAREA

*     EVALUATE THE J-TH CELL SOLUTE CONCENTRATION GRADIENTS.

      STARTX = RNUMEX - (CELLI * GRPCEL)
      SUM = 0.0
      DO 10 K = CELNUM, CELLI+1, -1
         SUM = SUM + CELLM(7, K, LVLCNT)
 10   CONTINUE

      X(1) = SUM
      DO 20 K = 1, GRPCEL-1
         X(K+1) = SUM + (K * HSTEPV(CELLI))
 20   CONTINUE

*        USING QUASI-HERMITE SPLINE, GENERATE MATRIX OF SPLINE
*        COEFFICIENTS.

         DO 40 K = 1, GRPCEL
            Y(K) = FLUXMM(STARTX+K)
 40      CONTINUE

         NX = GRPCEL
         IC = NGRPTS / NCELLS

         CALL IQHSCU(X, Y, NX, C, IC, IER)

*        INTEGRATE THE SPLINE OVER THE REQUIRED INTERVAL.

         A = X(1)
         B = X(GRPCEL)

         CALL DCSQDU(X, Y, NX, C, IC, A, B, Q, IER)

*        THE VALUE OF THE MASS OF DRY MATTER (MDM) IS
*        ESTIMATED FROM THE INTRACELLULAR VOLUME THE DENSITY
*        (APPROXIMATELY EQUAL TO THE DENSITY OF WATER)
*        AND THE PROPORTION OF DRY MATTER IN THE CELLULAR
*        VOLUME WHICH COMPRISES STARCH, PROTEINS, SOLUTES
*        EVALUATED TO 18% FOR STORED MATERIAL.

         MDM = VCO * 0.18 / DW

         T1 = - 2.0 * PI * CELLM(6, CELLI, LVLCNT) / MDM

*     FLAG TO INDICATE IF THE SYMPLAST TRANSPORT IS CONSIDERED.

      IF(FPLASM .EQ. 1) THEN

         CSTOM(1, CELLI) = T1 * Q
     &         - (ACPO * FLUXPM(CELLI, 1) / MDM)
     &         - (ACPO * FLUXPM(CELLI, 2) / MDM)

      ELSE

         CSTOM(1, CELLI) = T1 * Q

      ENDIF

      END
**********************************************************************
*                         SUBROUTINE OUTPUT                          *
**********************************************************************
*                                                                    *
*  PURPOSE   - THIS SUBROUTINE OUTPUTS THE RESULTS OF THE            *
*              CALCULATIONS IN SUITABLE FORM FOR ANALYSIS.           *
*                                                                    *
*  USAGE   - CALL OUTPUT(TIME, TSTEP, FLUXMM, FLUXPM, VELV, FLUXAM)  *
*                                                                    *
*  ARGUMENTS AND VARIABLES                                           *
*                                                                    *
*             TTIME - CURRENT TIME, IN SEC.                          *
*             TSTEP - CURRENT INTEGRATION TIME STEP, IN SEC.         *
*            FLUXMM - VECTOR OF TRANSMEMBRANE FLUXES, IN             *
*                     G CM-2 SEC-1.                                  *
*            FLUXPM - VECTOR OF PLASMODESMAL FLUXES, IN              *
*                     G CM-2 SEC-1.                                  *
*              VELV - VECTOR OF MASS AVERAGE VELOCITIES              *
*            FLUXAM - VECTOR OF APOPLASTIC FLUXES.                   *
*            STARTX - GRID POINT POSITION INDEX ON EXTENDED SPACE    *
*                     GRID.                                          *
*               SUM - SUMMATION VARIABLE.                            *
**********************************************************************
```

```
      SUBROUTINE OUTPUT(TTIME, TSTEP, TMAX, FLUXMM,
     &                  FLUXPM, VELV, FLUXAM, PCNT, PTEST, ITECNT)

      INTEGER NGRPTS, NCELLS, ITECNT, PCNT

      PARAMETER(NGRPTS = 3500, NCELLS = 100)

*     ARGUMENTS.

      REAL*4 TTIME, TSTEP, FLUXMM(0:NGRPTS),
     &       FLUXPM(NCELLS, 2), VELV(0:NGRPTS),
     &       FLUXAM(2, 0:NGRPTS, 3), PTEST

*     COMMON VARIABLES.

      COMMON /C1/ RNUM, RNUMEX, CELNUM, GRPCEL, COLNUM
      COMMON /C5/ SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &            ACPO, LCO, RIO, RCO, RBO, GTORT
      COMMON /C8/ HSTEPV(NCELLS), KSTEP
      COMMON /C4/ CDIFCM(0:(NGRPTS*2)-NCELLS)
      COMMON /C12/ CSIM(0:NGRPTS, 3), CSCM(4, NCELLS, 3),
     &             CELLM(8, NCELLS, 3),
     &             STAGEV(NCELLS), CAVG
      COMMON /C13/ NLEVEL, LVLCNT, GRPTI, CELLI
      COMMON /C15/ FPLASM, FAREA, TM, PINT, PPINT

      REAL*4 CDIFCM, HSTEPV, KSTEP, CSIM, CSCM, CELLM,
     &       NLEVEL, CAVG

      REAL*4 SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &       ACPO, LCO, RCO, RIO, RBO, GTORT, PPINT, TMAX

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL, TM,
     &        COLNUM, STAGEV, LVLCNT, GRPTI, CELLI, FPLASM, FAREA,
     &        PINT

*     ROUTINE VARIABLES.

      REAL*4 SUM

      INTEGER STARTX

*     OUTPUT CURRENT TIME AND CURRENT INTEGRATION TIME STEP, IN SEC.

      WRITE(2, 2000) TTIME, TTIME / 60.0, TSTEP

*     INTERSTITIUM VARIABLES:
*     OUTPUT CURRENT: POSITION INDEX, DISTANCE, SUCROSE
*     CONCENTRATION, APOPLAST FLUXES(DIFFUSIVE, CONVECTIVE, NET)
*     OF SUCROSE, NET FLUX OF WATER, AND WATER TRANSMEMBRANE FLUX.

      WRITE(2, *)
      WRITE(2, *)
      WRITE(2, *) ' INTERSTITIUM VARIABLES; EXTENDED GRID',
     &            ' POSITION; DISTANCE FROM THE CENTRE.'
      WRITE(2,*)
      WRITE(2,*)' ******************************************',
     &'**********************************************************',
     &'***********'
      WRITE(2,*)
      WRITE(2, 2005)
      WRITE(2,*)
      WRITE(2,*)' ******************************************',
     &'**********************************************************',
     &'***********'

      DO 10 K = 1, CELNUM

         WRITE(2, 2010) K
         SUM = 0.0
         DO 20 L = CELNUM, K, -1
            SUM = SUM + CELLM(7, L, LVLCNT)
 20       CONTINUE

         STARTX = RNUMEX - ((K - 1) * GRPCEL)

         DO 10 J = 0, GRPCEL-1
            IF ((K .EQ. 1) .AND. (J .EQ. 0)) THEN
              WRITE(2, 2020) SUM, CSIM( STARTX-J, LVLCNT),
     &   CDIFCM(2*(STARTX-J)-(CELNUM-K)),
     &   FLUXAM(2,STARTX-J,1), VELV(STARTX-J),
     &   FLUXAM(2,STARTX-J,3),
     &   FLUXAM(1,STARTX-J,3), FLUXMM(STARTX-J)

            ELSE
              WRITE(2, 2030) STARTX-J, SUM, CSIM(STARTX-J, LVLCNT),
     &   CDIFCM(2*(STARTX-J)-(CELNUM-K)),
     &   FLUXAM(2, STARTX-J,1), VELV(STARTX-J),
     &   FLUXAM(2, STARTX-J,3), FLUXAM(1, STARTX-J, 3),
     &   FLUXMM(STARTX-J)

            END IF
            SUM = SUM - HSTEPV(K)

 10   CONTINUE

*     INTRACELLULAR VARIABLES:
*     OUTPUT CURRENT: CELL GEOMETRICAL CHARACTERISTICS,
*     INTRACELLULAR CONCENTRATIONS AND PLASMODESMAL FLUXES IF
*     DESIRED.

      WRITE(2, *)
      WRITE(2, *)
      WRITE(2, *) ' GEOMETRICAL CHARACTERISTICS,',
     &            ' INTRACELLULAR CONCENTRATION OF WATER',
     &            ' AND PLASMODESMAL FLUXES IF DESIRED.'

      WRITE(2,*)
      IF (FPLASM .EQ. 1) THEN
      WRITE(2,*) ' SYMPLAST TRANSPORT IS CONSIDERED.'
      ELSE
      WRITE(2,*) ' SYMPLAST TRANSPORT IS NOT CONSIDERED.'
      ENDIF

      IF (FAREA .EQ. 1) THEN
      WRITE(2,*) ' AREA OF EXTRACELLULAR SPACE VARIES.'
      ELSE
      WRITE(2,*) ' AREA OF EXTRACELLULAR SPACE IS FIXED.'
      ENDIF
      DO 40 K = 1, CELNUM

         WRITE(2, 2100) K, STAGEV(K)
         WRITE(2, 2110)
         WRITE(2, 2120) (CELLM(1, K, LVLCNT)/VCO),
     &   (CELLM(2, K, LVLCNT)/VIO),
     &   (CELLM(3, K, LVLCNT)/VTO),
     &   (CELLM(4, K, LVLCNT)/RCO),
     &   (CELLM(5, K, LVLCNT)/RIO),
     &   (CELLM(6, K, LVLCNT)/RBO),
     &   (CELLM(7, K, LVLCNT)/LCO),
     &   (CELLM(8, K, LVLCNT)/AIO),
     &   CELLM(9, K, LVLCNT)
         WRITE(2, 2130)
         WRITE(2, 2140) (CSCM(I, K, LVLCNT), I = 1, 4),
     &                  (FLUXPM(K, L), L = 1, 2)
 40      CONTINUE

*     WRITING THE INTERMEDIATE PROFILES IF THE FLAG INDICATES

      IF(PINT .EQ. 1) THEN
      IF((TTIME .EQ. PPINT) .OR. (TTIME .EQ. TMAX)) THEN
      WRITE(4,*) NLEVEL
      WRITE(4,*) TTIME
      WRITE(4,*) TSTEP
      WRITE(4,*) KSTEP
      WRITE(4,*) LVLCNT
      WRITE(4,*) PCNT
      WRITE(4,*) PTEST
      WRITE(4,*) ITECNT

      DO 21 K = 1, CELNUM
      WRITE(4,*) STAGEV(K)
 21   CONTINUE

      DO 22 J = 0, RNUMEX
      DO 22 K = 1, 3
      WRITE(4,*) CSIM(J, K)
 22   CONTINUE

      DO 23 J = 1, CELNUM
      DO 23 K = 1, 3
      WRITE(4,*) CSCM(1, J, K)
      WRITE(4,*) CSCM(2, J, K)
      WRITE(4,*) CSCM(3, J, K)
      WRITE(4,*) CSCM(4, J, K)
 23   CONTINUE

      DO 24 J = 1, CELNUM
      DO 24 K = 1, 3
      WRITE(4,*) CELLM(1, J, K)
      WRITE(4,*) CELLM(2, J, K)
      WRITE(4,*) CELLM(3, J, K)
      WRITE(4,*) CELLM(4, J, K)
      WRITE(4,*) CELLM(5, J, K)
      WRITE(4,*) CELLM(6, J, K)
      WRITE(4,*) CELLM(7, J, K)
      WRITE(4,*) CELLM(8, J, K)
      WRITE(4,*) CELLM(9, J, K)
 24   CONTINUE
      PPINT = PPINT + PPINT
      ELSE
      ENDIF
      ELSE
      ENDIF

*     FORMATS

 2000 FORMAT(//, '  CURRENT TIME: ',F10.4,' SEC, ', F8.4,' MIN ', /,
     &          '  CURRENT INTEGRATION TIME STEP (SEC): ', F7.4)
 2005  FORMAT(T6,'INDEX',T18,'Z',T30,'CSUC',T41,'Dcor',T54,'JS',
     &        T65,'v',T78,'NS',T90,'NW',T101,'RWM')
 2010  FORMAT(/, 2X, 'CELL INDEX: ', I5 )
 2020  FORMAT(T4, 'SURFACE', 3X, E12.5, 2X, F10.3, 6(2X, E10.3))
 2030  FORMAT(T4, I5, 5X, E12.5, 2X, F10.3, 6(2X, E10.3))
 2100  FORMAT(/, 4X, 'CELL POSITION INDEX: ',I5, 4X,
     &             'DEHYDRATION STAGE: ',I3 )
 2110  FORMAT(T7, 'VC', 10X, 'VI', 10X, 'VT', 10X, 'RC', 10X, 'RI',
     &        10X, 'RB', 10X, 'LC', 10X, 'AI', 10X, 'IRESP')
 2120  FORMAT(9(2X, E10.3))
 2130  FORMAT(T7, 'XT', 10X, 'XST', 8X, 'XP', 8X,
     &        'XV', 10X, 'JP-', 10X, 'JP+')
 2140  FORMAT(6(2X, E10.3))

      END
```

```
************************************************************************
*                         PROGRAM EXPCAL                               *
************************************************************************
*                                                                      *
*  PURPOSE  - THIS SUBROUTINE EVALUATES THE SUCROSE, WATER             *
*             CONCENTRATION AND THE DENSITY FOR EACH CELL IN ORDER     *
*             TO BE ABLE TO COMPARE THE THEORETICAL AND                *
*             THE EXPERIMENTAL PROFILES AT A CERTAIN TIME.             *
*  THIS PROGRAM IS USED AFTER THE SIMULATION OF THE PROGRAM            *
*  M.TISSUE.FOR HAS BEEN PERFORMED.                                    *
************************************************************************

      INTEGER NGRPTS, NCELLS, PCNT,ITECNT

      PARAMETER(NGRPTS=3500, NCELLS=100)

      REAL*4 PMVV(2), RT, PMV, PPV, TTIME, NLEVEL,
     &       SPVFO, WVFO, VOIDFO, VCO, VIO, VTO, AIO, ACMO,
     &       ACPO, LCO, RIO, RCO, RBO, GTORT, CAVG, KSTEP, TSTEP,
     &       EMODCO(2),WRESF,PCO, GRTOL, GRSTEP, CNTOL,
     &       DIFCV, POLCOM(0:2), COMPFV(3), DDM, DW,
     &       CSIM(0:NGRPTS,3), CSCM(4,NCELLS,3), CELLM(8,NCELLS,3),
     &       NSTEPV(NCELLS), PTEST

      REAL*4 TSTEPO, TSTEPM, TMAX, TPRINT, IRESFO

      REAL*4 CSBOV, CSIOV, XTO, XSTO, XPO, XVO, MWV(2),MDMC,MDME,
     &       WG,WF,WS,WKP,WKS,WST,WP,MG,MF,MKP,MKS

      INTEGER RNUM, RNUMEX, CELNUM, GRPCEL,
     &       COLNUM, ITEMAX, STAGEV(NCELLS), DEGV, FPLASM, FAREA,
     &       LVLCNT,CELLI

      REAL*4 TEMP, R, TSAREA, THICKO, DIAMCO, RPLASM, PI
      DATA PI/3.14159/

      INTEGER TOTCEL

      REAL*4 DIAMTO, PPINT

      INTEGER NX, IC, IER, TM, PINT

      REAL*4 A, B, O, X(NGRPTS/NCELLS),Y(NGRPTS/NCELLS),
     &       C(NGRPTS/NCELLS,3)

      REAL*4 SC(NCELLS), SE(NCELLS), ST(NCELLS), WT(NCELLS),
     &       WE(NCELLS), WC(NCELLS), MTE(NCELLS), MTC(NCELLS),
     &       MT(NCELLS), PERSUC(NCELLS), PERWAT(NCELLS),
     &       DENS(NCELLS)

      REAL*4 SUM

      INTEGER STARTX

*     INPUT DATA

*     SOLUTION CHARACTERISTICS

      READ(1, *) (PMVV(I), I = 1, 2)
      WRITE(2, *) ' PMVV: ', (PMVV(I), I = 1, 2)
      READ(1, *) (MWV(I), I = 1, 2)
      WRITE(2, *) ' MWV: ', (MWV(I), I = 1, 2)
        READ(1, *) DIFCV, DEGV, (POLCOM(J), J = 0, DEGV)
        WRITE(2, *) ' DIFCV, DEGV, POLCOM: ', DIFCV, DEGV,
     &                  (POLCOM(J), J = 0, DEGV)

*     OSMOTICUM CHARACTERISTICS

      READ(1, *) TEMP, R
      WRITE(2, *) ' TEMP, R: ', TEMP, R
*
*     EVALUATE THE RT CONSTANT
      RT = R * (TEMP + 273.15)
      WRITE(2,*) ' RT: ',RT
      READ(1,*) CSBOV
      WRITE(2,*) ' CSBOV: ',CSBOV

*     INITIAL TISSUE CHARACTERISTICS (FULL TURGOR TISSUE)

      READ(1, *) TSAREA, THICKO, DIAMCO
      WRITE(2, *) ' SEMI-INFINITE MEDIUM GEOMETRY CONSIDERED '
      WRITE(2, *) ' TSAREA, THICKO, DIAMCO: ', TSAREA, THICKO,
     &               DIAMCO
      READ(1, *) GTORT, SPVFO, WVFO
      WRITE(2, *) ' GTORT, SPVFO, WVFO: ', GTORT, SPVFO, WVFO

*     CALCULATE THE INITIAL TISSUE VOID FRACTION
      VOIDFO = SPVFO + WVFO
      WRITE(2,*) ' VOIDFO: ',VOIDFO

      READ(1,*) FPLASM
         IF(FPLASM .EQ. 1) THEN
            WRITE(2,*) ' SYMPLAST TRANSPORT IS CONSIDERED '
         ELSE
            WRITE(2,*) ' SYMPLAST TRANSPORT IS NOT CONSIDERED '
         ENDIF
      READ(1,*) FAREA
         IF(FAREA .EQ. 1) THEN
            WRITE(2,*) ' THE AREA OF EXTRACELLULAR SPACE VARIES'
         ELSE
            WRITE(2,*) ' THE AREA OF EXTRACELLULAR SPACE IS FIXED'
         ENDIF

*     CELL CHARACTERISTICS

      READ(1, *) WRESF, RPLASM
      WRITE(2, *) ' WRESF, RPLASM: ', WRESF, RPLASM

*     CALCULATE THE INITIAL RESISTANCE OF THE INTERSTITIUM COMPLEX
      IRESFO = (SPVFO + (WVFO * WRESF)) / VOIDFO
      WRITE(2,*) ' IRESFO: ',IRESFO

      READ(1, *) (EMODCO(K), K = 1, 2)
      WRITE(2, *) ' LINEAR VARIATION OF ELASTIC MODULUS',
     &              ' CONSIDERED: ', (EMODCO(K), K = 1, 2)
      READ(1,*) PCO
      WRITE(2,*) ' PCO: ',PCO
      READ(1, *) (COMPFV(K), K = 1, 3)
      WRITE(2, *) ' COMPLIANCE FACTOR VALUES: ',
     &             (COMPFV(K), K = 1, 3)
```

```
      READ(1, *) PMV
      WRITE(2, *) ' PMV: ', PMV
      READ(1, *) PPV
      WRITE(2, *) ' PPV: ', PPV
      READ(1, *) XTO, XSTO, XPO, XVO
      WRITE(2, *) ' XTO: ', XTO,' XSTO: ',XSTO,' XPO: ',XPO,
     &            ' XVO: ', XVO
      READ(1,*) WG,WF,WS,WKP,WKS,WST,WP
      WRITE(2,*) ' WG: ',WG,' WF: ',WF,' WS: ',WS,' WKP: ',WKP,
     &            ' WKS: ',WKS,' WST: ',WST,' WP: ',WP
      READ(1,*) MG,MF,MKP,MKS
      WRITE(2,*) ' MG: ',MG,' MF: ',MF,' MKP: ',MKP,' MKS: ',MKS
      READ(1,*) DDM,DW
      WRITE(2,*) ' DDM: ',DDM,' DW:',DW

*     INTERSTITIUM CHARACTERISTICS

      READ(1, *) CSIOV
      WRITE(2, *) ' CSIOV: ', CSIOV

*     CALCULATION OF CAVG USING A CORRELATION RELATING
*     THE CONCENTRATION OF SUCROSE IN THE INTERSTITIUM

      CAVG = (((1.0029 + (0.3689 * CSIOV)) +
     &        (1.0029 + (0.3689 * CSBOV))) / 2
      WRITE(2,*) ' CAVG: ', CAVG

*     PARAMETERS REQUIRED BY GEARS AND CRANK-NICOLSON ROUTINES

      READ(1, *) GRTOL, GRSTEP, CNTOL, ITEMAX
      WRITE(2, *) ' GRTOL, GRSTEP, CNTOL, ITEMAX: ', GRTOL, GRSTEP,
     &              CNTOL, ITEMAX
      READ(1, *) GRPCEL
      WRITE(2, *) ' GRPCEL: ', GRPCEL
      READ(1, *) TSTEPO, TSTEPM, TMAX, TPRINT
      WRITE(2, *) ' TSTEPO, TSTEPM, TMAX, TPRINT: ', TSTEPO, TSTEPM,
     &              TMAX, TPRINT
      READ(1, *) TM, PINT, PPINT
      WRITE(2, *) ' TM, PINT, PPINT: ', TM, PINT, PPINT

*     GET INITIAL EQUIVALENT CYLINDRICAL UNIT CELL MENSURATIONS

*     INITIAL CELLULAR VOLUME

      DATA PI/3.14159/
      VCO = (PI * (DIAMCO**3)) / 6.0

*     INITIAL TOTAL UNIT CELL VOLUME

      VTO = VCO / (1.0 - VOIDFO)

*     INITIAL INTERSTITIUM VOLUME

      VIO = VTO - VCO
      WRITE(2, *) ' VCO, VIO, VTO: ', VCO, VIO, VTO

*     INITIAL CELL MEMBRANE SURFACE AREA.

      ACMO = (1.0 - RPLASM) * PI * (DIAMCO**2)

*     INITIAL FRACTIONAL PLASMODESMAL TRANSFER AREA.

*     NOTE:  THE TERM "PLASMODESMAL TRANSFER AREA" USED
*            THROUGHOUT THE PROGRAM REFERS TO THE FRACTION OF
*     TOTAL PLASMODESMAL AREA WHICH IS USED, FOR ANY GIVEN CELL,
*     TO DESCRIBE THE SURFACE AVAILABLE FOR SYMPLASTIC TRANSPORT
*     TO/FROM ADJOINING CELLS. THIS FRACTION IS ASSUMED EQUAL FOR
*     ALL 6 POINTS OF CONTACT

      ACPO = (RPLASM * ACMO) / (6.0 * (1.0 - RPLASM))

*     INITIAL LENGTH OF UNIT CYLINDRICAL CELL

      LCO = (6.0 * VTO * (GTORT**(3.0 / 2.0)) / PI)**(1.0 / 3.0)

*     INITIAL RADIUS OF INTERSTITIUM CYLINDER

      RIO = ACMO / (2.0 * PI * LCO)

*     INITIAL CELL CYLINDER RADIUS

      RCO = SQRT((VCO / (PI * LCO)) + (RIO**2))

*     INITIAL BUFFER CYLINDER RADIUS

      RBO = SQRT((RIO**2) - (VIO / (PI * LCO)))
      WRITE(2, *) ' LCO, RIO, RCO, RBO: ', LCO, RIO, RCO, RBO

*     INITIAL INTERSTITIUM APOPLASTIC TRANSFER AREA

      AIO = PI * ((RIO**2) - (RBO**2))
      WRITE(2, *) ' AIO, ACMO, ACPO: ', AIO, ACMO, ACPO

*     DEFINE SOME PARAMETERS TO BE USED BY CRANK-NICOLSON ALGORITHM

*     GET INITIAL AVERAGE UNIT CELL DIAMETER

      DIAMTO = (6.0 * VTO / PI)**(1.0 / 3.0)
      WRITE(2, *) ' DIAMTO: ', DIAMTO

*     EVALUATE TOTAL NUMBER OF CELLS IN TISSUE

      TOTCEL = INT((TSAREA * THICKO / VTO) + 1.0)
      WRITE(2, *) ' TOTCEL: ', TOTCEL

*     EVALUATE NUMBER OF EQUIVALENT CYLINDRICAL UNIT CELLS IN
*     MODEL COLUMN.

*     CELNUM IS TAKEN AS THE NEAREST INTEGER GREATER THAN
*     THE CALCULATED VALUE (SEE CELNUM DEFINITION).

      CELNUM = INT((THICKO / DIAMTO) + 1.0)

*     EVALUATE NUMBER OF COLUMNS IN THE STUDIED TISSUE.

      COLNUM = TOTCEL / CELNUM

*     EVALUATE TOTAL NUMBER OF SPACE GRID POINTS (FOR BOTH SPACE
*     GRIDS).
```

```
      RNUM = (CELNUM * GRPCEL) - CELNUM
      RNUMEX = (CELNUM * GRPCEL) - 1
      WRITE(2, *) ' CELNUM, COLNUM, RNUM, RNUMEX: ', CELNUM, COLNUM,
     &            RNUM, RNUMEX

*     READ THE FILE.
      READ(3,*) NLEVEL
      READ(3,*) TTIME
      READ(3,*) TSTEP
      READ(3,*) KSTEP
      READ(3,*) LVLCNT
      READ(3,*) PCNT
      READ(3,*) PTEST
      READ(3,*) ITECNT

      DO 11 K = 1, CELNUM
      READ(3,*) STAGEV(K)
 11   CONTINUE

      DO 12 J = 0, RNUMEX
      DO 12 K = 1, 3
      READ(3,*) CSIM(J, K)
 12   CONTINUE

      DO 13 J = 1, CELNUM
      DO 13 K = 1, 3
      READ(3,*) CSCM(1, J, K)
      READ(3,*) CSCM(2, J, K)
      READ(3,*) CSCM(3, J, K)
      READ(3,*) CSCM(4, J, K)
 13   CONTINUE

      DO 14 J = 1, CELNUM
      DO 14 K =1, 3
      READ(3,*) CELLM(1, J, K)
      READ(3,*) CELLM(2, J, K)
      READ(3,*) CELLM(3, J, K)
      READ(3,*) CELLM(4, J, K)
      READ(3,*) CELLM(5, J, K)
      READ(3,*) CELLM(6, J, K)
      READ(3,*) CELLM(7, J, K)
      READ(3,*) CELLM(8, J, K)
      READ(3,*) CELLM(9, J, K)
 14   CONTINUE

*     OUTPUT CURRENT TIME AND CURRENT INTEGRATION TIME STEP, IN SEC.

      WRITE(2, 2000) TTIME, TTIME / 60.0, TSTEP

*     INTERSTITIUM VARIABLES:
*     OUTPUT CURRENT: POSITION INDEX, DISTANCE, SUCROSE
*     CONCENTRATION, APOPLAST FLUXES(DIFFUSIVE, CONVECTIVE, NET)
*     OF SUCROSE, NET FLUX OF WATER, AND WATER TRANSMEMBRANE FLUX.

      WRITE(2, *)
      WRITE(2, *)
      WRITE(2, *) ' INTERSTITIUM VARIABLES; EXTENDED GRID',
     &            ' POSITION; DISTANCE FROM THE CENTRE.'
      WRITE(2,*)
      WRITE(2,*)' ****************************************',
     &'*****************************************************',
     &'***********'
      WRITE(2,*)
      WRITE(2, 2005)
      WRITE(2,*)
      WRITE(2,*)' ****************************************',
     &'*****************************************************',
     &'***********'

      DO 81 K = 1, CELNUM
      HSTEPV(K) = CELLM(7, K, LVLCNT) / REAL(GRPCEL-1)
 81   CONTINUE

      DO 101 K = 1, CELNUM

         WRITE(2, 2010) K
         SUM = 0.0
         DO 201 L = CELNUM, K, -1
            SUM = SUM + CELLM(7, L, LVLCNT)
 201     CONTINUE

         STARTX = RNUMEX - ((K - 1) * GRPCEL)

         DO 101 J = 0, GRPCEL-1
            IF ((K .EQ. 1) .AND. (J .EQ. 0)) THEN
              WRITE(2, 2020) SUM, CSIM( STARTX-J, LVLCNT)

            ELSE
              WRITE(2, 2030) STARTX-J, SUM, CSIM(STARTX-J, LVLCNT)

            ENDIF
            SUM = SUM - HSTEPV(K)

 101   CONTINUE

*     INTRACELLULAR VARIABLES:
*     OUTPUT CURRENT: CELL GEOMETRICAL CHARACTERISTICS,
*     INTRACELLULAR CONCENTRATIONS AND PLASMODESMAL FLUXES IF
*     DESIRED.

      WRITE(2, *)
      WRITE(2, *)
      WRITE(2, *) ' GEOMETRICAL CHARACTERISTICS,',
     &            ' INTRACELLULAR CONCENTRATION OF WATER',
     &            ' AND PLASMODESMAL FLUXES IF DESIRED.'

      WRITE(2,*)
      IF (FPLASM .EQ 1) THEN
      WRITE(2,*) ' SYMPLAST TRANSPORT IS CONSIDERED.'
      ELSE
      WRITE(2,*) ' SYMPLAST TRANSPORT IS NOT CONSIDERED.'
      ENDIF

      IF (FAREA .EQ. 1) THEN
      WRITE(2,*) ' AREA OF EXTRACELLULAR SPACE VARIES.'
      ELSE
      WRITE(2,*) ' AREA OF EXTRACELLULAR SPACE IS FIXED.'
      ENDIF

      DO 40 K = 1, CELNUM
```

```
         WRITE(2, 2100) K, STAGEV(K)
         WRITE(2, 2110)
         WRITE(2, 2120) (CELLM(1, K, LVLCNT)/VCO),
     &    (CELLM(2, K, LVLCNT)/VIO),
     &    (CELLM(3, K, LVLCNT)/VTO),
     &    (CELLM(4, K, LVLCNT)/RCO),
     &    (CELLM(5, K, LVLCNT)/RIO),
     &    (CELLM(6, K, LVLCNT)/RBO),
     &    (CELLM(7, K, LVLCNT)/LCO),
     &    (CELLM(8, K, LVLCNT)/AIO),
     &    CELLM(9, K, LVLCNT)
         WRITE(2, 2130)
         WRITE(2, 2140) (CSCM(I, K, LVLCNT), I = 1, 4)
 40      CONTINUE

*     ESTIMATION OF THE MASS OF DRY MATTER OF THE CELLULAR VOLUME.

      MDMC = VCO * 0.18 / DW

*     ESTIMATION OF THE MASS OF DRY MATTER OF THE EXTRACELLULAR
*     VOLUME.

      MDME = VIO * 0.03 / DW

*     CALCULATION OF THE SUCROSE CONCENTRATION,
*     THE WATER CONTENT AND THE MASS OF CELLULAR VOLUME
*     FOR EACH CELL AND STORED THEM IN A VECTOR.

      DO 10 J = 1, CELNUM
      CELLI = J
      STARTX = RNUMEX - (CELLI * GRPCEL)

      SC(CELLI) = WS / ((CSCM(1,CELLI, LVLCNT)/DW)
     &           + (1.0 / DDM))

      WC(CELLI) = CSCM(1, CELLI, LVLCNT)
     &   / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0/DDM))

      MTC(CELLI) = (CSCM(1,CELLI, LVLCNT) + 1.0) * MDMC

*     CALCULATION OF THE AVERAGE SUCROSE CONCENTRATION OF
*     THE EXTRACELLULAR VOLUME OF THE CELL PUT THEM IS A VECTOR
*     AS WELL AS THE CONCENTRATION OF WATER AND THE MASS OF
*     EXTRACELLULAR SPACE.

      SUM = 0.0
      DO 20 K=CELNUM, CELLI+1, -1
      SUM = SUM + CELLM(7, K, LVLCNT)
  20  CONTINUE

      X(1) = SUM
      Y(1) = CSIM(STARTX+1, LVLCNT)
      DO 30 K = 1, GRPCEL-1
      X(K+1) = X(K) + HSTEPV(CELLI)
      Y(K+1) = CSIM(STARTX+1+K, LVLCNT)
  30  CONTINUE

*     USING A QUASI HERMITE SPLINE, GENERATE THE MATRIX OF
*     SPLINE COEFFICIENTS.

      NX = GRPCEL
      IC = NGRPTS/NCELLS

      CALL IQHSCU(X, Y, NX, C, IC, IER)

*     INTEGRATE THE SPLINE OVER THE REQUIRED INTERVAL.
      A = X(1)
      B = X(GRPCEL)

      CALL DCSQDU(X, Y, NX, C, IC, A, B, Q, IER)

      SE(CELLI) = Q / CELLM(7, CELLI, LVLCNT)

      WE(CELLI) = CAVG - SE(CELLI)

      MTE(CELLI) = (CAVG * CELLM(2, CELLI, LVLCNT))+ MDME

      MT(CELLI) = MTC(CELLI) + MTE(CELLI)

      ST(CELLI) = ((CELLM(1,CELLI,LVLCNT) * SC(CELLI))
     &        + (CELLM(2, CELLI, LVLCNT) * SE(CELLI)))
     &        / CELLM(3, CELLI, LVLCNT)

      WT(CELLI) = ((CELLM(1,CELLI,LVLCNT) * WC(CELLI))
     &        + (CELLM(2, CELLI, LVLCNT) * WE(CELLI)))
     &        / CELLM(3, CELLI, LVLCNT)

      PERSUC(CELLI) = ((SE(CELLI)*CELLM(2,CELLI,LVLCNT))
     &        + (SC(CELLI)*CELLM(1,CELLI,LVLCNT))) / MT(CELLI)

      PERWAT(CELLI) = (((CAVG-SE(CELLI)) * CELLM(2,CELLI, LVLCNT))
     &        + (WC(CELLI)* CELLM(1, CELLI,LVLCNT)))
     &        / MT(CELLI)

      DENS(CELLI) = (((SC(CELLI) +
     &    (WST / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WP / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WKP / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WKS / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WS / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WG / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM)))
     &    +(WF / ((CSCM(1,CELLI, LVLCNT)/DW) + (1.0 / DDM))))
     &     * CELLM(1,K,LVLCNT)) + (SE(CELLI) * CELLM(2,K,LVLCNT))
     &     + (WC(CELLI)* CELLM(1,K,LVLCNT))
     &     + (WE(CELLI)* CELLM(2,K,LVLCNT)))
     &     / CELLM(3,K, LVLCNT)

  10  CONTINUE

*     WRITING THE RESULTS.

      WRITE(2,*)
      WRITE(2,*)
      WRITE(2,*) '  VALUE OF SUCROSE, WATER CONCENTRATION',
     &  ' DENSITY OF EACH CELL IN DIFFERENT UNITS.'
      WRITE(2,*)

      DO 25 K = 1, CELNUM
      WRITE(2,2100) K, STAGEV(K)
      WRITE(2,2150)
      WRITE(2,2160) SC(K),SE(K),ST(K),WC(K),WE(K),WT(K)
      WRITE(2,2170)
      WRITE(2,2180) MTC(K),MTE(K),MT(K),PERSUC(K),PERWAT(K),DENS(K)
      WRITE(2,2190)
      WRITE(2,2200) CELLM(1, K, LVLCNT),CELLM(2, K, LVLCNT),
     &          CELLM(3, K, LVLCNT), MDMC, MDME
 25   CONTINUE

2000 FORMAT(//, '  CURRENT TIME: ',F10.4,' SEC, ', F9.4,' MIN.', /,
     &        '  CURRENT INTEGRATION TIME STEP (SEC): ', F7.4)
2005  FORMAT(T6,'INDEX',T19,'Z',T30,'CSUC')
2010  FORMAT(/, 2X, 'CELL INDEX: ', I5 )
2020  FORMAT(T4, 'SURFACE', 3X, E10.3, 2X, E10.3)
2030  FORMAT(T4, I5, 5X, E12.5, 2X, F10.3)
2100  FORMAT(/, 4X, 'CELL POSITION INDEX: ',I5, 4X,
     &        'DEHYDRATION STAGE: ',I3 )
2110  FORMAT(T7, 'VC', 10X, 'VI', 10X, 'VT', 10X, 'RC', 10X, 'RI',
     &       10X, 'RB', 10X, 'LC', 10X, 'AI', 10X, 'IRESF')
2120  FORMAT(8(2X, E10.3))
2130  FORMAT(T7, 'XT', 10X, 'XST', 8X, 'XP', 8X,
     &        'XV', 10X)
2140  FORMAT(4(2X, E10.3))
2150  FORMAT(T7,'SC',10X,'SE',10X,'ST',10X,'WC',10X,'WE',10X,'WT')
2160  FORMAT(6(2X,E10.3))
2170  FORMAT(T7,'MTC',10X,'MTE',10X,'MT',8X,'PERSUC',7X,
     &        'PERWAT',10X,'DENS')
2180  FORMAT(6(2X,E10.3))
2190  FORMAT(T7,'VC',10X,'VI',10X,'VT',10X,'MDMC',10X,'MDME')
2200  FORMAT(T7,5(2X,E10.3))

      END
```